Analytical and innovative solutions for heat transfer problems involving phase change and interfaces

Finite element solution for diffusion–convection problems with isothermal phase changes

Une approche éléments finis pour la simulation de problèmes de diffusion–convection induisant des transformations isothermes

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ABSTRACT

A finite element algorithm is proposed to simulate steady-state diffusion–convection problems with isothermal phase changes. This technique is based on an enthalpic approach discretized by means of a finite element approximation of the enthalpy including the latent heat of transformation. The interface of phase changes is implicitly described without coupling with an interface-capturing technique. An example clearly shows the efficiency of the method developed.

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RÉSUMÉ

Un algorithme éléments finis est proposé pour simuler les problèmes de diffusion–convection avec des changements de phase isothermes. Cette technique repose sur une approche en enthalpie, discrétisée au moyen d'une approximation éléments finis de l'enthalpie intégrant la chaleur latente de transformation. L'interface est décrite de manière implicite sans couplage avec une technique spécifique de capture d'interface. Un exemple met clairement en évidence l'efficacité de la méthode développée.

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1. Introduction

Finite element analysis of heat transfer involving phase changes is a numerical problem which has been extensively studied in the past years. Steady-state conduction–convection with a phase change occurs in many engineering processes. One example is welding processes which are widely used in the material processing industry. For example, welding processes or heat treatments involve a very small size heat source compared to that of the structure studied. Local modeling of the thermal and mechanical effects requires very fine meshes in the vicinity of the source so as to perform a finite element analysis. A refined analysis of the joint may lead to significant size problems. This can be avoided by means of a re-meshing procedure refining discretization in the vicinity of the heat source only along the weld joint. This type of transient analysis involves long calculation times and it is very often assumed that a quasi-steady state is established when the structure

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displays a translation geometry on a long distance. In order to determine the temperature field during the steady phase of the process, it only takes a steady analysis with a reference connected with the source velocity. That is why the models are very often based on diffusion–convection formalism as described in [1]. It makes it possible to significantly simplify the simulations by doing away with the transient state analysis whose calculation time is very long. With this new reference, the material moves owing to the thermo-mechanical load and partial time derivatives are canceled.

It is well-known that the finite element simulation of phase changes is confronted with computational pathologies when high latent heat effects appear. For example, these phenomena can occur during directional solidification for crystal growth applications [2,3] or solidification phenomena for continuous casting process which is widely used in the material processing industry [4]. It is necessary to find the temperature field of a casting and the location of the solid/liquid interface in order to understand and control such a process and to improve the quality of products. The accuracy of the temperature field and interface location is very important because it directly affects the calculated thermal stresses and velocities of fluid flow.

One of the most famous solution methods is the fixed grid technique well described in [5] and [6]. In this way, the latent heat effect can be easily overcome with an equivalent heat capacity [7–9]. The application of this technique raises problems since the phase change is spread over a small range of temperatures as for isothermal phase changes. One may easily numerically miss the very high (virtually infinite) peak of heat capacity, thus failing to respect exact conservation of energy.

To overcome these difficulties, an enthalpic formulation has been introduced by Feulvarch et al. for the modeling of transient and steady-state diffusion–convection problems [10]. The proposed approach 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 technique for steady-state diffusion–convection problems with a discontinuous finite element approximation of the enthalpy in space such as proposed in [11] for transient heat conduction problems. The advantages of the method developed in this paper are two-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).

The article is organized as follows. Section 2 is devoted to the general formulation of the problems envisaged and the enriched numerical scheme proposed is detailed in Section 3. The example proposed in Section 4 shows evidence the potential and the efficiency of the method proposed.

2. Steady-state diffusion–convection problem

The problem studied in this paper is based on the formulation proposed by Feulvarch and Bergheau [10] for stationary convection–diffusion problems:

For $i = 1, 2$, find functions T_i, H_i defined on Ω_i verifying the boundary value problem defined by

$$\begin{cases} \vec{v} \cdot \overrightarrow{\text{grad}} H_i = \text{div}(\lambda \overrightarrow{\text{grad}} T_i) & \text{in } \Omega_i \\ T_i = g(H_i) & \text{in } \Omega_i \\ \lambda \overrightarrow{\text{grad}} T_i \cdot \vec{n} = q^{(p)} + k(T^{(p)} - T_i) & \text{on } \partial\Omega_i \\ T_i = T_m & \text{on } \partial\Omega_m \\ \lambda \overrightarrow{\text{grad}} T_2 \cdot \vec{n}_m - \lambda \overrightarrow{\text{grad}} T_1 \cdot \vec{n}_m = \Delta H \vec{v} \cdot \vec{n}_m & \text{on } \partial\Omega_m \end{cases} \quad (1)$$

In these equations, $\partial\Omega_m$ is the common portion of the boundaries of the open sets Ω_1 and Ω_2; $\partial\Omega_i = (\overline{\Omega}_i \backslash \Omega_i) \backslash \partial\Omega_m$ as shown in Fig. 1; $\vec{v}$ is the material velocity in the reference frame of work; λ is the thermal conductivity which can be temperature dependent; g is the function providing the temperature in terms of the enthalpy[1] as shown in Fig. 2; $\vec{n}$ is the unit outward normal vector to the boundary; $\vec{n}_m$ is the unit outward normal vector to Ω_1 on the boundary $\partial\Omega_m$; $q^{(p)}$ 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 $k \rightarrow +\infty$). The isothermal phase change is assumed to take place at temperature T_m on the smooth surface $\partial\Omega_m$.

The weak formulation of the problem is classically obtained by multiplying Eq. $(1)_1$ by a weighting function T_i^*, Eq. $(1)_2$ by a weighting function H_i^*, for $i = 1, 2$, and integrating over both domains Ω_1 and Ω_2, respectively. Integrating the first equation by parts and accounting for the boundary condition $(1)_3$, one thus obtains the following variational formulation of the problem:

For $i = 1, 2$, find functions T_i, H_i such as for all functions T_i^*, H_i^*,

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[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.
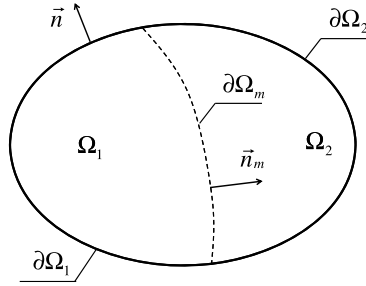
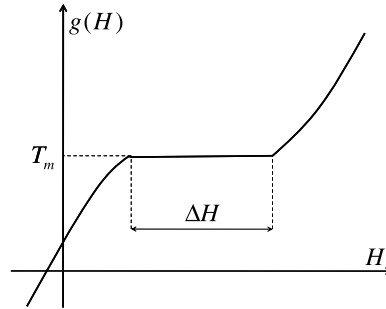**Fig. 1.** Schematic representation of the domain Ω and the interface of phase change $\partial\Omega_m$.

Fig. 2. Typical evolution of the function $g(H)$ for an isothermal transformation occurring at temperature T_m with a latent heat $\triangle H$.

$$\begin{cases} \displaystyle\int_{\Omega_i} \vec{v} \cdot \overrightarrow{\mathrm{grad}} H_i T_i^* \,\mathrm{d}V + \int_{\Omega_i} \lambda \overrightarrow{\mathrm{grad}} T_i \cdot \overrightarrow{\mathrm{grad}} T_i^* \,\mathrm{d}V + \int_{\partial\Omega_i} k T_i T_i^* \,\mathrm{d}S - \int_{\partial\Omega_i} \big(q^{(p)} + k T^{(p)}\big) T_i^* \,\mathrm{d}S = 0 \\[2ex] \displaystyle\int_{\Omega_i} \big[T_i - g(H_i)\big] H_i^* \,\mathrm{d}V = 0 \end{cases} \tag{2}$$

with

$$\lambda \overrightarrow{\mathrm{grad}} T_2 \cdot \vec{\mathrm{n}}_m - \lambda \overrightarrow{\mathrm{grad}} T_1 \cdot \vec{\mathrm{n}}_m = \triangle H \vec{v} \cdot \vec{\mathrm{n}}_m \quad \text{and} \quad T_1 = T_2 = T_m \quad \text{on } \partial\Omega_m \tag{3}$$

Under the boundary conditions (3), the enthalpy H is discontinuous in space throughout the interface of phase change $\partial\Omega_m$. Thus, H can be expressed as the sum of a continuous function h and a discontinuous one providing the enthalpy of transformation $\triangle H = H_2 - H_1$ due to the phase change:

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

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

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

This definition includes the release or the storage of latent heat and therefore the discontinuity of the heat flux throughout the interface of phase change. These considerations allow to define the following weak formulation on the whole domain Ω, from a mathematical point of view:

Find functions $T \in H^1(\Omega)$, $H = h + \mathcal{I}_d \triangle H \in L^2(\Omega)$ *such as for all functions* $T^* \in H^1(\Omega)$, $H^* \in L^2(\Omega)$,

$$\begin{cases} \displaystyle\int_{\Omega} \frac{\mathrm{d}H}{\mathrm{d}t} T^* \,\mathrm{d}V + \int_{\Omega} \lambda \overrightarrow{\mathrm{grad}} T \cdot \overrightarrow{\mathrm{grad}} T^* \,\mathrm{d}V + \int_{\partial\Omega} k T T^* \,\mathrm{d}S - \int_{\partial\Omega} \big(q^{(p)} + k T^{(p)}\big) T^* \,\mathrm{d}S = 0 \\[2ex] \displaystyle\int_{\Omega} \big[T - g(H)\big] H^* \,\mathrm{d}V = 0 \end{cases} \tag{4}$$

Despite the fact that the gradient of the function H is not defined on $\partial\Omega_m$, it is possible mathematically to express the derivative in time of the enthalpy $\frac{\mathrm{d}H}{\mathrm{d}t}$ by a convective term in this integral formulation. Indeed, $H = h + \mathcal{I}_d \triangle H \in L^2(\Omega)$, the integrals are taken in the sense of Lebesgue and the $(N+1)$-dimensional measure of the N-dimensional boundary $\partial\Omega_m$ is zero. However, the gradient of enthalpy is not suitable to represent the jump in enthalpy $\triangle H$ throughout the boundary $\partial\Omega_m$ from the physical point of view. This is the reason why the derivative is denoted with the general symbol $\frac{\mathrm{d}}{\mathrm{d}t}$.

3. Finite element formulation

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

$$T(\vec{x}) = \sum_{i=1}^{N} T_i N_i(\vec{x}) \quad \in H^1(\Omega) \tag{5}$$

In this expression, N denotes the number of nodes, T_i the value of the function T at node i and $N_i(\vec{x})$ the shape function associated to this node. 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 used as proposed in [11]:

$$H(\vec{x}) \approx H^d(\vec{x}) = \sum_{i=1}^{N} h_i N_i(\vec{x}) + \mathcal{I}_d \Delta H \quad \in L^2(\Omega) \tag{6}$$

Following Galerkin's standard approach, the test functions T^* and H^* are taken in the same form. Substituting the nodal approximations (5) and (6) into the variational formulation (4), one obtains the following non-linear system of equations:

$$\begin{cases} [\mathbf{K}] \cdot \{\mathbf{T}\} + \{\mathbf{C}^d\} - \{\mathbf{F}\} = \{\mathbf{0}\} \\ [\mathbf{M}] \cdot \{\mathbf{T}\} - \{\mathbf{G}\} = \{\mathbf{0}\} \end{cases} \tag{7}$$

where $\{\mathbf{T}\} \equiv (T_i)_{1\leqslant i\leqslant N}$, $\{\mathbf{h}\} \equiv (h_i)_{1\leqslant i\leqslant N}$ denote the vectors of nodal values of the functions T and h. $[\mathbf{K}] \equiv (K_{i,j})_{1\leqslant i,j\leqslant N}$, $[\mathbf{M}] \equiv (M_{i,j})_{1\leqslant i,j\leqslant N}$, $\{\mathbf{F}\} \equiv (F_i)_{1\leqslant i\leqslant N}$ and $\{\mathbf{G}\} \equiv (G_i)_{1\leqslant i\leqslant N}$ are respectively matrices and vectors which are described in [11] for transient heat conduction problems. The vector $\{\mathbf{C}^d\} \equiv (C_i^d)_{1\leqslant i\leqslant N}$ is defined by

$$C_i^d \equiv \int_{\Omega} \frac{dH^d}{dt} N_i \, dV \tag{8}$$

We have already seen that it is not possible to define the material derivative of the enthalpy from a single convective term based on the gradient of enthalpy because it is discontinuous. This is also true for the discontinuous approximation of the enthalpy proposed above. To overcome this difficulty, we propose to introduce an auxiliary approximation of the enthalpy H^c of class C^1 on Ω for the resolution. Considering that H^c is continuous unlike H^d, the gradient of H^c is able to model all spacial evolutions of the enthalpy. This approximation H^c is taken equal to the discontinuous approximation H^d in a weak sense. One can note that the function H^d is not defined on the boundary $\partial\Omega_m$ but it is possible mathematically to define this weak equality on Ω. As mentioned before, the integrals are taken in the sense of Lebesgue and the $(N + 1)$-dimensional measure of the N-dimensional boundary $\partial\Omega_m$ is zero. To compute the material derivative in time by means of a convective term depending on the gradient of H^c, we establish the following result:

Proposition 1. *In a steady-state configuration*:

$$\forall \delta H^c \in H^1(\Omega), \quad \int_{\Omega} \delta H^c (H^c - H^d) \, dv = 0 \quad \implies \quad \int_{\Omega} \delta H^c \left(\frac{dH^c}{dt} - \frac{dH^d}{dt} \right) dv = 0 \tag{9}$$

Proof. It is clear that:

$$\forall \delta H^c, \quad \int_{\Omega} \delta H^c (H^c - H^d) \, dv = 0 \quad \implies \quad \frac{d}{dt} \int_{\Omega} \delta H^c (H^c - H^d) \, dv = 0$$

Applying the Leibniz–Reynolds' transport theorem in a steady state, we get:

$$\frac{d}{dt} \int_{\Omega} \delta H^c (H^c - H^d) \, dv = \int_{\partial\Omega} \delta H^c (H^c - H^d) \vec{v} \cdot \vec{n} \, ds$$

From the divergence theorem, we can write:

$$\int_{\partial\Omega} \delta H^c (H^c - H^d) \vec{v} \cdot \vec{n} \, ds = \int_{\Omega} \left(\text{div}(\delta H^c \vec{v}) \right) (H^c - H^d) \, dv + \int_{\Omega} \delta H^c \left(\vec{v} \cdot \overrightarrow{\text{grad}} H^c - \vec{v} \cdot \overrightarrow{\text{grad}} H^d \right) dv$$

Thus, under the equality defined in a weak sense between H^c and H^d, since $\delta H^c \in H^1(\Omega)$ and assuming that $\vec{v}$ is sufficiently regular, we get in a stationary configuration:
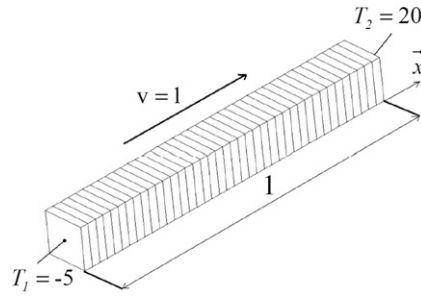
Fig. 3. Boundary conditions.

$$\forall \delta H^c, \quad \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \delta H^c \big(H^c - H^d \big) \, \mathrm{d}v = \int_\Omega \delta H^c \bigg(\frac{\mathrm{d}H^c}{\mathrm{d}t} - \frac{\mathrm{d}H^d}{\mathrm{d}t} \bigg) \mathrm{d}v \qquad \square$$

One can note that the steady material derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ is taken equal to $\vec{\mathrm{v}} \cdot \overrightarrow{\mathrm{grad}}$. This is mathematically correct even if this definition is not satisfactory for H^d from the physical point of view as mentioned in Section 2.

Considering this result and a classical finite element approximation for H^c (as for the temperature T), system (7) becomes

$$\begin{cases} [\mathbf{K}] \cdot \{\mathbf{T}\} + [\mathbf{C}] \cdot \{\mathbf{H}\} - \{\mathbf{F}\} = \{\mathbf{0}\} \\ [\mathbf{M}] \cdot \{\mathbf{T}\} - \{\mathbf{G}\} = \{\mathbf{0}\} \end{cases} \tag{10}$$

where $\{\mathbf{H}\} \equiv (H_i)_{1 \leqslant i \leqslant N}$ denotes the vector of nodal values of H^c; $[\mathbf{C}] \equiv (C_{i,j})_{1 \leqslant i,j \leqslant N}$ is a matrix defined by

$$C_{i,j} \equiv \int_\Omega N_i \vec{\mathrm{v}} \cdot \overrightarrow{\mathrm{grad}} N_j \, \mathrm{d}V \tag{11}$$

Eqs. (10) are solved by a Newton–Raphson iterative method as described in [11] for transient heat conduction problems. One can note that the standard Galerkin's approach can lead to spurious oscillations for convection-dominated problems [12]. To obtain stable solutions, various techniques can be used such as sub-grid methods [13–15] or the so-called Streamline upwind/Petrov–Galerkin [16] as used in [10].

4. Application to the Stefan problem

This application is a non-dimensional example which consists of modeling a one-dimensional isothermal transformation with a constant velocity along x axis as shown in Fig. 3. The temperatures are set to $T_1 = -5$ and $T_2 = 20$ for $x = 0$ and $x = 1$, respectively.

The material properties are:

– Specific heat: $C = 1$;
– Mass density: $\rho = 1$;
– Thermal conductivity: $\lambda = 1$;
– Latent heat: $L = 70$;
– Temperature of transformation: $T_m = 0$.

The finite element mesh is composed of linear elements. The element size Δx is uniform and taken equal to 0.1. Fig. 4 shows the computed temperature and enthalpy distributions, together with the analytical temperature distribution given in [4]. The numerical results closely agree with the analytical distribution.

5. Conclusion

The aim of this article was to detail a numerical algorithm to simulate latent heat effects during isothermal transformations for steady-state diffusion–convection configurations. This technique is based on an enthalpic formulation of the heat equation coupled with a function providing the temperature from the enthalpy. In this approach, the discretization is based on a classical finite element approximation of the temperature and the enthalpy which includes the jump of enthalpy throughout the interface of phase changes. This interface is implicitly described without coupling with an interface-capturing technique as for usual X-FEM applications. An example clearly shows the efficiency of the method developed.
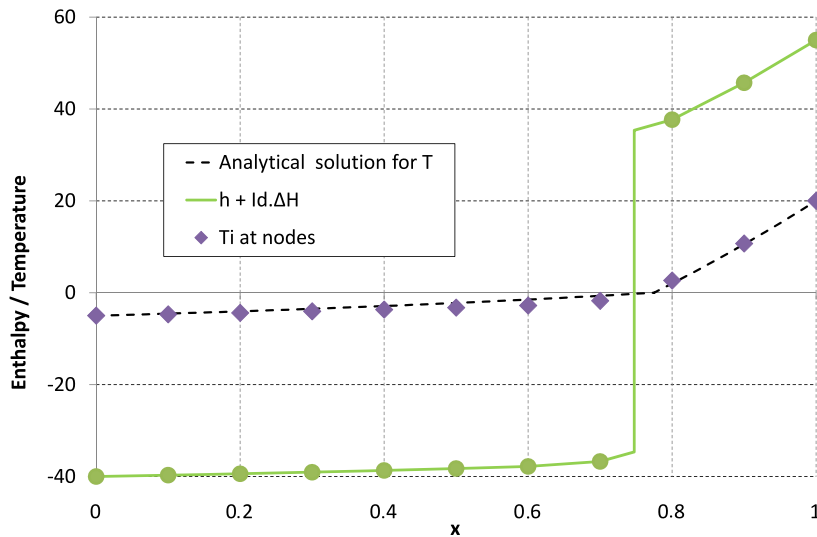
Fig. 4. Temperature and enthalpy distributions.

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