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An enthalpy based heat equation to solve the phase change

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1. Introduction

In a materials, the phase change induces a discontinuity in the enthalpy H quantified by the latent heat L. A lot of methods were developed to model this phenomena, resumed in [1]. The last one was proposed by Feulvarch [2]. Its original idea is to proceed with the known curve temperature T versus enthalpy H, whose derivative is never infinite. This approach is solved simultaneously in temperature and enthalpy thanks to an implicit time discretisation and a Newton-Raphson linearisation.

This method allows to solve the famous Stefan problem by a very effective way. Particularly, the time step can be larger than with an effective specific heat formulation. This last formulation is numerically penalized by the infinite derivative of solid fraction versus temperature during phase change. The other usual formulation, called enthalpy method [3], is based on the heat equation written in terms of enthalpy. To obtain such a formulation, the heat equation is processed from temperature to enthalpy by the function enthalpy versus temperature. Even there, this leads to infinite derivative, and so to the numerical problems associated.

However, the formulation proposed by Feulvarch has a larger memory cost. Indeed, two variables (*H* and *T*) have to be saved permanently. We propose, in this paper, to rewrite this formulation to avoid the use of temperature variable. The results is strictly the same, but the memory cost is usual, since only the enthalpy is saved.

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2. Methods

According to [2], the heat equation is written as following:

$$\frac{\partial H}{\partial t} - \mathrm{div}\left(k\,\mathbf{grad}\,T\right) = 0 \quad \text{and} \quad T = g(H) \tag{1}$$

The fields temperature *T* and enthalpy *H* are defined on space time $\Omega \times [0, t_{end}]$, and the function *g(H)* is supposed to be known, and its derivative exists for all *H*. After taking into account of boundary conditions, and after the finite element discretisation and time implicit scheme (the equation is multiplied by the time increment *dt*), we obtain:

$$[\boldsymbol{M}]\{\boldsymbol{H}\} + dt[\boldsymbol{K}]\{\boldsymbol{T}\} - \{\boldsymbol{f}\} = \{\boldsymbol{0}\} \quad \text{and} \quad [\boldsymbol{M}]\{\boldsymbol{T}\} - [\boldsymbol{M}]\{\boldsymbol{g}\} = \{\boldsymbol{0}\} \tag{2}$$

where the terms of the vector $\{\boldsymbol{g}\}$ are the nodal values $g_i(t) = g(H_i(t))$ since, following the finite element approximation, with the shape function $N_i(\boldsymbol{x})$:

$$g(H(\boldsymbol{x},t)) = g\left(\sum_i N_i(\boldsymbol{x}) H_i(t)\right) \approx \sum_i N_i(\boldsymbol{x}) g(H_i(t)) = \sum_i N_i(\boldsymbol{x}) g_i(t) \tag{3}$$

The equations (2) are solved by a Newton-Raphson linearization, as follows:

$$\begin{bmatrix} dt[\boldsymbol{K}] & [\boldsymbol{M}] \\ [\boldsymbol{M}] & -[\boldsymbol{M}][\boldsymbol{L}] \end{bmatrix} \begin{Bmatrix} \boldsymbol{dT} \\ \boldsymbol{dH} \end{Bmatrix} = - \begin{Bmatrix} [\boldsymbol{M}]\{\boldsymbol{H}\} + dt[\boldsymbol{K}]\{\boldsymbol{T}\} - \{\boldsymbol{f}\} \\ [\boldsymbol{M}]\{\boldsymbol{T}\} - [\boldsymbol{M}]\{\boldsymbol{g}\} \end{Bmatrix} \tag{4}$$

where the matrix $[\boldsymbol{L}]$ arises of the derivative of $\{\boldsymbol{g}\}$ at $\{\boldsymbol{H}\}$, that means:

$$[\boldsymbol{L}]_{ij} = \frac{\partial g_i}{\partial H_j} = \frac{\partial g(H_i)}{\partial H_j} = \begin{cases} g'(H_i) \\ 0 \quad \text{if } i \neq j \end{cases} \tag{5}$$

Hence, $[\boldsymbol{L}]$ is a diagonal matrix. The second equation of (4) allows to find easily $\{\boldsymbol{dT}\}$:

$$\{\boldsymbol{dT}\} = \{\boldsymbol{g}\} - \{\boldsymbol{T}\} + [\boldsymbol{L}]\{\boldsymbol{dH}\}$$

and, the first one, the enthalpy increment $\{\boldsymbol{dH}\}$:

$$([\boldsymbol{M}] + dt[\boldsymbol{K}][\boldsymbol{L}])\{\boldsymbol{dH}\} = -[\boldsymbol{M}]\{\boldsymbol{H}\} + \{\boldsymbol{f}\} - dt[\boldsymbol{K}]\{\boldsymbol{g}\} \tag{6}$$

This results is the Feulvarch's one, with a slight difference on the vector $\{\boldsymbol{g}\}$ definition. Now, substituting the second equation (1) in the first one:

$$\frac{\partial H}{\partial t} - \operatorname{div}(k\,\mathbf{grad}\, g(T)) = 0$$

So, the discretisation leads to the system (with the same notations):

$$[\boldsymbol{M}]\{\boldsymbol{H}\} + dt[\boldsymbol{K}]\{\boldsymbol{g}\} - \{\boldsymbol{f}\} = \{\boldsymbol{0}\}$$

Finally, its Newton-Raphson linearization gives exactly the same equation (6). The assembly procedure for the right hand side allows to avoid the storage of the complete vector $\{\boldsymbol{g}\}$. Only $\{\boldsymbol{H}\}$ is saved in memory.

3. Results

This formulation is applied to a classical Stephan Problem. Results are very effective and fast compared to usual approaches. The enthalpy-alone formulation can be extended to the case of a non-linear conductivity, if it is expressed as a function of enthalpy, and not temperature: *k(H)*.

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