2D solidification and melting model using FEM and adaptive meshing

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Abstract

In the case of pure materials, a precise modeling of solidification and melting phenomena may be achieved by controlling accurately the position and shape of the solidification front. We analyze two approaches. The first one considers a cylindrical ingot in which solid and liquid materials are present. The second one considers a piece of material melting in an infinite bath composed of the same melted material. In the first case, the static energy equation is written in term of enthalpy, and laminar liquid movements are expressed with velocity and pressure unknowns. The finite element mesh is adapted by moving internal nodes on a fixed mesh topology. A particular interface element has been introduced on the solidification front line. A Petrov Galerkin upwind scheme has been programmed. In the second case, transient energy equation is written in temperature. Fluid movements are introduced by exchange coefficients on the boundary. The displacements of the boundary line are controlled by a balance equation between the different thermal flux term: convection exchange term with fluid, internal flux, heat flux due to melting or solidification. An adaptation of the mesh is done in two ways: deformation of a given mesh or re-meshing.

List of symbols:

\[ T \] : temperature  \quad \hat{U}_s : stirring velocity
\[ L \] : latent heat of fusion  \quad \hat{U}_w : withdrawing velocity
\[ H \] : enthalpy  \quad \hat{n} : normal vector
\[ \rho \] : density  \quad \hat{V} : velocity of mesh
\[ k \] : thermal conductivity  \quad \vec{F} : external force density
\[ \alpha \] : thermal diffusivity  \quad Q_{th} : external power density
\[ h \] : heat transfer coefficient  \quad T_r : room temperature
1 Introduction

In the continuous casting processes for the elaboration of pure materials like silicon it is necessary to control the position and the shape of the solidification front. On the same way, in steel metallurgy processes like cored wire injection techniques, the difficulty is to make the good choice of the feed rate at given temperature and given depth of a ladle. The knowledge of the exterior solidification front position during time will permits to obtain the total melting time and adjust the speed of injection. For that the study of heat transfer at the phase change have to be as precise as possible. For such calculations, a lot of time steps are necessary. So particular attention is done to reduce as small as possible the CPU time of algorithms. To solve problem of phase change two kinds of methods can be applied: global methods or explicit methods with localization of solid liquid interface. In first methods only one domain is considered (liquid and solid) [2], [3]. The liquid solid interface is determined at the end of calculation. In the second methods 2 domains are modeled: the liquid and the solid regions [4], [5]. At the interface of these regions we take into account a continuity equation of heat flux with latent heat of phase change. In our case we choose the second method with moving boundary. This paper presents two numerical simulations of phase changes with two boundary models using the finite element method on our FLUX-EXPERT package [6].

2 Phase change models in continuous casting

We study the case of electromagnetic continuous casting of a cylindrical ingot in a cold crucible. The general physical problems in such processes result of coupling phenomena between electromagnetism, thermal and hydrodynamic equations. The electromagnetism creates sources for thermal and hydrodynamic phenomena. We present here a thermo-hydraulic model to take in account the latent heat given at the solid interface with moving boundary.

2.1 Physical equations and boundary conditions

Considering an axi-symmetrical geometry a 2D model has been developed. The problem is written in a fixed system of coordinates. We study a fixed volume constituted by the liquid meniscus and a part of the solid ingot fig.1. In this process the material is introduced in the top and withdraws in the bottom.
2.1.1 Thermo-hydraulic coupling with enthalpy

The energy equation is written in terms of total enthalpy. The temperature appears like a property of the enthalpy. The coupling is done by the way of the stirring velocity. The velocity has two components. The equations are:

\[ \rho (\vec{U}_w + \vec{U}_s) \nabla H = \nabla \cdot (k \nabla T) + Q_{th} \]  
\[ \rho (\vec{U}_s, \nabla) \vec{U}_s = -\nabla P + \mu_t \nabla^2 \vec{U}_s + \vec{F} \]  
\[ \nabla \cdot \vec{U}_s = 0 \]

The flow driven by electromagnetic stirring is turbulent. The Reynolds number is around 6000. The model is based on a global turbulent viscosity chosen, for an equivalent laminar flow characterised by Reynolds number around 200.

2.1.2 Boundary conditions

In this coupling we have two domains liquid and solid. The thermal problem is solved in both domains, and the velocities are calculated only in the liquid one.

The thermal boundary conditions of the problem are radiative mode on the meniscus ($\Gamma_{in}$), convective mode on the meniscus and on the vertical boundary ($\Gamma_{in}$), cold material entry at the top ($\Gamma_{in}$) and a condition of homogeneous Neumann on the symmetrical axis. At the liquid solid interface, for a pure material the unknown enthalpy is discontinuous.

The velocity boundary conditions are:

- $\vec{U}_s \cdot \vec{n} = 0$ on the meniscus and on the symmetrical axis,
- tangential stress equal to zero on the meniscus and on the symmetrical axis,
- logarithmic law on the solidification front.

2.2 Numerical model for enthalpy formulation

The study domain is divided in two regions. The liquid and solid regions are meshed in quadrangular elements. Along the solidification front we use special elements: interfacial elements. The interfacial element is a linear element with double point (same coordinates and different values for the unknowns) fig. 2. So
it is possible to impose boundary condition on these elements. In our case we impose the liberation of latent heat on these elements.

2.2.1 Mesh deformation

The use of these interfacial elements requires the knowledge of the exact position of the solidification front. But this position is unknown. So it is necessary to modify the position of the solidification front at each step of calculation. For this reason we chose a method of mesh deformation.

We define a deformation zone around the interface fig. 3. The displacement of the interfacial line is imposed by the boundary condition. The other nodes on the deformation zone are displaced by homothety in vertical direction.

At the beginning we imposed a first position of the liquid solid interface. After each step of calculation the shape of the solidification front is modified like this:

- The liberation of latent heat must be imposed for the enthalpy of the solidus $H_s$. At each step, the calculated enthalpy at the interface is different to the solidus enthalpy. So we displace each node of the interfacial element toward the line of isovalue $H_s$.
- The convergence is assumed when the interfacial line is along the value $H_s$.

2.2.2 F.E.M. Formulation

To solve this problem we use a Galerkin projective method. The enthalpy and velocity unknowns are interpolated on order 2 Lagrange elements $N_i$. The pressure is interpolated on order 0 Lagrange elements. The convection term is
unstable so we apply the S.U.P.G method (Stream Upwind Petrov Galerkin) [7]. This upwind term is tensorial. The weak formulation for the enthalpy equation is:

\[
\int_{\Omega} N_i \rho \vec{U}_s \cdot \vec{\nabla} H d\Omega - \int_{\Gamma_{\text{out}}} k \frac{dT}{dH} \vec{N}_i \vec{\nabla} H d\Gamma_{\text{out}} + \int_{\Gamma_{\text{in}}} N_i \rho \vec{U}_w \cdot \vec{n}_{\text{out}} H d\Gamma_{\text{in}} + \int_{\Omega} \gamma_{\text{upw}} (\vec{U}_w + \vec{U}_s) \cdot \vec{\nabla} N_i \rho (\vec{U}_w + \vec{U}_s) \cdot \vec{\nabla} H d\Omega = - \int_{\Gamma_{\text{in}}} N_i \rho \vec{U}_w \cdot \vec{n}_n H_{\text{in}} d\Gamma_{\text{in}} - \int_{\Gamma_{\text{in}}} \gamma_{\text{upw}} (\vec{U}_w + \vec{U}_s) \cdot \vec{\nabla} N_i Q_{\text{th}} d\Omega
\]

2.3 Application

We used this numerical model in the case of continuous casting of silicon. We present a comparison between the results obtained with this model and an experimental result on the figure 4. We can see an example of mesh deformation.

![Figure 4: Comparison between numerical results and experimental results](image)

The shape obtained with the numerical model is in good agreement with the experimental result under the same conditions. The temperature has a good homogeneity in the liquid and important gradients can be observed in the solid domain near the solidification front. The fluid flow is constituted by one toroidal vortex as it can be observed during the experiment. The maximal velocity is around 0.1 m/s. This value is similar to Alfvén velocity (0.35 m/s).
3 Phase change models in injection processes

We present here a 2D version of a 1D model initially developed for the simulation of cored wire injection processes [1]. A typical 2D geometry corresponds to a slice of a 3D object, moving rapidly in a bath. It may content different components. The coordinate system is assumed to be fixed to the slice plan. In the approach proposed here, only the melting or solidification on the boundary will be taken into account. The mesh is time evolutionary in geometry and topology.

3.1 Physical equations and boundary conditions

We consider a general study domain as described in Figure 5.

\[
\frac{\partial T}{\partial t} + \vec{V}(-\alpha \vec{V}T) = 0 \tag{4}
\]

On the exterior boundary heat transfer are considered all around the slice. The general equations (5) describe the external boundary conditions.

\[
\begin{align*}
    k \frac{\partial T}{\partial n} &= -h(T_{\text{surface}} - T_{\text{bath}}) - \rho L \frac{dR}{dt} \\
    T_{\text{surface}} &= T_{\text{melting}}
\end{align*}
\tag{5}
\]

The heat coefficients depend on the type of wire motion in the bath. In the case of a cylindrical wire with a transverse motion in the fluid, the exchange coefficient \( h \) expresses as:

\[
h = \frac{Nu \, k}{D}
\]

where, the Nusselt number \( Nu \) expression is:
The typical length scale $D$ is the diameter of the wire with:

$$Re = \frac{VD}{\nu} : \text{Reynolds number}$$

$$Pr = \frac{\nu}{\alpha} : \text{Prandt number with } \alpha, \text{ thermal diffusivity of the liquid}$$

In the case of injection, we have to use the average Nusselt number:

$$Nu = 0.43 + 0.19 Re^{0.6} Pr^{0.3}$$

Where $D$, typical length scale is the penetration depth. $D$ is at first sight unknown; nevertheless, the transfer coefficient is not very sensitive to the value of $D$. Consequently fixing a good order of magnitude to $D$ is sufficient.

### 3.2 Numerical model

The general domain is meshed automatically with triangular or quadrangular elements using Delaunay algorithm. We use order 2 finite elements with Lagrange polynomials for interpolation. By this way we can get a good representation of the moving boundary with few nodes. Integration is calculated with Gauss method.

#### 3.2.1 Mesh evolution in time

As in the 1D model, we can evaluate a displacement of each boundary node at any time according to equations (5). In fact, the internal flux and the convection flux are known. It is then possible to calculate the displacement of each node along the normal of the boundary. Some problems have to be solved. Firstly, when working with order 2 Lagrange elements it is necessary to ensure a good position of the second order nodes of the boundary elements. In the case of a circular shape of the domain with a constant exchange coefficient $h$, the position of nodes will be perfectly controlled. In the case of irregular geometry shape of the boundary and space variation of $h$, it will be necessary to correct the position during simulation time. For that we have developed a Catmull-Rom spline fitting algorithm [8] which is applied to all the boundary points.

The second problem due to the displacements of boundary nodes, is the adaptation of the interior mesh. We propose three different solutions:

a) Displacement of the order 2 interior nodes in the vicinity of the boundary. This solution is very fast but may fail due to the existence of flat or reversed elements. It appears when the boundary is reaching order 1 interior nodes.

b) Displacement of all interior nodes. Each order 1 interior node is moved to the gravity center of its connected elements. Order 2 nodes are re-calculated. This solution will permit to follow without trouble the movements of the boundary. It is more expensive in term of CPU time than solution a.
c) Re-meshing of the domain: this algorithm very expensive, must be used only when re-distribution of nodes along the boundary is necessary, particularly when the curvature is important.

In cases a and b, we introduce a transport term in the equation (4) with a speed of mesh coefficient. It will be calculated on each Gauss integration point of each finite element. This speed is interpolated directly from the velocity value of each element node with Lagrange polynomials.

Thermal equation (4) becomes:

\[ \frac{\partial T}{\partial t} + \vec{V} \cdot \vec{\nabla} T + \vec{\nabla} (\alpha \vec{\nabla} T) = 0 \]  

(6)

### 3.2.2 Finite element formulation

The Galerkin projection is applied to equation (6). The weak discretized form is:

\[ \int_{\Omega} N_i T'' d\Omega + \Delta t \int_{\Omega} \vec{V} \cdot \vec{\nabla} T d\Omega + \Delta t \int_{\Omega} \alpha \vec{\nabla} N_i \cdot \vec{\nabla} T d\Omega = \int_{\Omega} N_i T'' d\Omega \]  

(7)

Equation (5) establishes a Dirichlet condition on each boundary node.

### 3.2.3 Resolution algorithm

The general algorithm is transient and non-linear. For stability in time, implicit method is used. For stability in space, SUPG Petrov Galerkin upwind scheme is applied on the transport term [7]. Finite difference scheme is used for time decomposition.

Normal vectors are calculated on order 2 nodes. Order 1 node normal vectors are obtained by averaging both order 2 node normal vectors in the vicinity and normalizing it (fig.6).

```
Algorithm:
Initiate the temperature on the domain
For (each time step)
1. Calculate the temperature in solid solving equation (7)
2. Calculate normal gradients and vectors on the boundary
3. Displacements = 0
4. Do while (T and Displacement not converged)
   a. Calculate Displacement with equation (5)
   b. Update the mesh (ref. 3.2.1 a. or b.)
```

![Figure 6: Calculation of normal vectors to boundary](image-url)
3.3 Application

We consider a square piece of steel (diagonal 2cm) injected at high velocity in a steel bath. To test the influence of a non-uniform motion in the bath, we have chosen a variable exchange coefficient \( h \) on the boundary. \( h \) value is varies linearly from 100000 W/m² on right side, to 10000 W/m² on the left side. Figure 7 presents results obtained at different times. At the beginning a crust of frozen metal of the bath is growing all around the slice. After 1 sec melting it begins to reduce on the right hand, while at the same time the left side is still increasing. At 2.3 sec, both sides are melting.

4 Conclusion

Two different finite element approaches for melting control of pure material have been presented. The physical models of both simulations were strongly different. The first one is based on Enthalpy method and treats fluid dynamics problem, with a moving interface only along vertical direction. The second considers a boundary moving freely. It appears clearly that each model can be transformed to integrate characteristics of the other. Typically in the first one, free moving boundary algorithm may be introduced, and in the second one interfacial elements may have interest also on the boundary. In both cases, future trends will be full automatic adaptive meshing, coupling with concentration equations and 3D analyses.

References:


Figure 7: An example of steel melting with heterogeneous exchange coefficient