Two-Phase Approach for Solidification Problems: Modelling the Mushy Zone Deformation
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Abstract
This paper exposes the development of a two-phase model accounting for mass, momentum and energy transfer, especially dedicated to the analysis of the thermo-mechanical behavior of metallic alloys in the mushy state. Macroscopic balance equations are first derived from local ones by the use of a spatial averaging method. Constitutive equations of both the liquid and the solid phases as well as interfacial exchange terms are then expressed by the mean of phenomenological considerations. Lastly, the resolution strategy is detailed.

Introduction
During solidification, a metallic alloy can be either in the liquid, solid or mushy (semi-solid) state. In the mushy state, the solid phase may form a coherent skeleton through which the liquid may flow. The solid and the liquid may then deform in different manner, what will result in variations of the composition of the final product. In order to describe this phenomena and be able to predict the final properties of parts, the mushy alloy has to be considered as a two-phase medium, made of a solid and a liquid phase that may have different velocities. A two-phase material is heterogeneous by nature, the morphology and spatial distribution of the phases it is made of being generally random and complex. A direct resolution of equilibrium equations at the microscopic level would therefore require huge computing times which are not suited for the simulation of the casting of industrial parts. In order to be able to describe the thermo-mechanical evolution of a whole part during solidification, local equations therefore have to be replaced by “macroscopic” ones. After reminding the basics of the spatial averaging method (section 2), a first set of macroscopic balance equations is presented (section 3), under the assumption of macroscopic isotropy of the microstructure, suited for equiaxed dendritic solidification. The full determination of the model then requires constitutive assumptions that are discussed in sections 4 and 5. Lastly, a resolution strategy is proposed (section 6).

Spatial averaging method
In this work, we adopt the spatial averaging method [1]-[5], which consists in assuming that the macroscopic behavior of the two-phase medium is governed by the average of local equations taken on a volume $V_0$. The size of this elementary representative volume is supposed to be small compared to the size of the studied part, but large enough compared to the interfacial structures size. The spatial averaging method is now rather classical so we will only remind its basis in this first section, limiting our presentation to the case of a two-phase saturated medium made of a solid phase (index $s$) and a liquid one (index $l$). Let us consider, as illustrated in Figure 1, a fixed volume of material $V_0$. Each phase $k$ occupies the volume $V_k$, and the average of a scalar quantity $u_k$ associated to phase $k$ is called macroscopic quantity and reads:
\[
\langle u_k \rangle = \frac{1}{V_0} \int_{V_k} u_k \, dV = \frac{1}{V_0} \int_{V_0} \chi_k u_k \, dV
\]
where $\chi_k$ is the characteristic function of phase $k$ which value is 1 in volume $V_k$ and 0 elsewhere. The intrinsic volume average of $u_k$ in phase $k$, will be denoted either $\langle u_k \rangle^k$ or $u^k$:
\[
u^k = \langle u_k \rangle^k = \frac{1}{V_k} \int_{V_0} u_k \chi_k \, dV
\]
For $u_k=1$, we obtain from (1) the definition of the volume fraction of phase $k$, $g_k$ as
\[ g_k = \frac{1}{V_0} \int_{V_0} Z_k dV = \frac{V_k}{V_0} \tag{3} \]
and the assumption of saturated medium immediately yields
\[ g_s + g_l = 1 \tag{4} \]
According to previous definitions (1)-(3), we get the relation between $\langle u_k \rangle$ and $u^k$:
\[ \langle u_k \rangle = g_k u^k \tag{5} \]
The fluctuating component of $u_k$ is defined as
\[ \hat{u}_k = (u_k - u^k) \chi_k \tag{6} \]
It thus represents the variation of $u_k$ around its intrinsic average value. This notation enables to express the intrinsic average of the product of two variables $u_k$ and $v_k$ as
\[ \langle u_k v_k \rangle^k = \langle u_k \rangle^k \langle u_k \rangle^k + \langle \hat{u}_k \hat{v}_k \rangle^k \tag{7} \]
Finally, the following averaging theorems relating the average of a derivative to the derivative of the average can be proved (e.g. [4] or [5]):
\[ \left\langle \frac{\partial u_k}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle u_k \rangle - \frac{1}{V_0} \int_A u_k (\mathbf{w} \cdot \mathbf{n}_k) dS = \frac{\partial}{\partial t} \langle u_k \rangle - \langle u_k (\mathbf{w} \cdot \mathbf{n}_k) \rangle^* \tag{8} \]
\[ \langle \nabla u_k \rangle = \nabla \langle u_k \rangle + \frac{1}{V_0} \int_A u_k \mathbf{n}_k dS = \nabla \langle u_k \rangle + \langle u_k \mathbf{n}_k \rangle^* \tag{9} \]
where surface $A$ is the interface between solid and liquid, $\mathbf{w}$ the local velocity of this interface, and $\mathbf{n}_k$ is the outward normal vector to volume $V_k$ (see Figure 1). Since we only consider the case of two phases, please notice that for each point of surface $A$, we have $\mathbf{n}_s = -\mathbf{n}_l$. In this last equation, the following notation was introduced, as done in [5]:
\[ \langle u_k \rangle^* = \frac{1}{V_0} \int_A u_k dS \tag{10} \]

Table 1: Microscopic conservation equations of phase $k$.

<table>
<thead>
<tr>
<th></th>
<th>$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = 0$</th>
<th>$\frac{\partial (\rho_k \mathbf{v}_k)}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k \otimes \mathbf{v}_k) = \nabla \cdot \mathbf{f}_k - \nabla p_k + \rho_k \mathbf{g}$</th>
<th>$\frac{\partial (\rho_k h_k)}{\partial t} + \nabla \cdot (\rho_k h_k \mathbf{v}_k) + \nabla \cdot \mathbf{q}_k = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Momentum</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td><strong>Energy</strong></td>
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</tbody>
</table>
Macroscopic two-phase formulation

Phases microscopic thermo-mechanical evolution is assumed to be governed by the classical continuous media equilibrium equations, that is to say mass, momentum and energy balances, summarized in Table 1. Both phases are assumed to be incompressible materials at the microscopic scale and their constitutive equations are written as

\[ \sigma_k = -p_k \delta + s_k \]  

where \( p_k \) denotes the hydrostatic pressure and \( s_k \) is the deviatoric part of stress tensor \( \sigma_k \). The incompressibility assumption makes more relevant the description of the energy equation by the mean of enthalpy \( h_k \) balance (13). Please notice that for simplicity, viscous heat dissipation, compression work and volumetric energy sources are not included. Those assumption could be easily relaxed but seem appropriate for most practical solidification problems.

Making use of the averaging theorems and of the assumption of macroscopic isotropy, the integration of local equations (11)-(13) over \( V_0 \) leads to the corresponding macroscopic ones summarized in Table 2, where velocity vector \( V^k \) stands for the average velocity \( \langle v_k \rangle \). As mentioned in [4], the strict application of averaging rules leads to more complicated results where fluctuation terms may intervene. For simplicity, equations (16) to (18) are obtained under the assumption that fluctuating components are negligible with respect to their corresponding intrinsic value. Particularly, we assume that

\[ \hat{\rho}_k << \rho^k \quad \text{and} \quad \|\hat{v}_k\| << \|v^k\| \]  

Besides, \( \hat{\rho} \) is assumed constant in the solidification interval and the additional inertia terms due to mass transfer are neglected in eq. (17).

Due to the averaging process, integrals over the interfacial area \( A \) arise, thus leading to additional terms \( \Gamma_k, M_k \) and \( Q_k \), that respectively account for mass, momentum and energy exchanges with the other phase. Their expression, presented in Table 3, will be discussed in next sections. Those quantities are subjected to interfacial balance equations summarized in Table 3, obtained assuming that no sources are likely to be created on interface \( A \) (e.g.: no surface tension between phases).

### Table 2: Macroscopic conservation equations of phase \( k \).

| Mass | \( \rho^k \frac{d g_{k}}{dt} + \rho^k \nabla \cdot \hat{v}^k = \Gamma_k \) |
| Momentum | \( \rho^k \frac{d v^k}{dt} + \rho^k \nabla \cdot \left( \frac{1}{g_k} v^k \otimes v^k \right) = \nabla \cdot \langle s_k \rangle - \nabla \cdot \langle p_k \rangle + g_k \rho^k \sigma + M_k \) |
| Energy | \( \rho^k \frac{d (g_k h^k)}{dt} + \rho^k \nabla \cdot (h^k \hat{v}^k) + \nabla \cdot \langle q_k \rangle = Q_k \) |

### Table 3: interfacial balances – exchange terms

| Mass | \( \Gamma_k = -\langle \rho_k (v_k - w) \cdot n_k \rangle^* \) |
| Momentum | \( M_k = \langle \sigma_k \cdot n_k \rangle^* \) |
| Energy | \( Q_k = -\langle \rho_k h_k (v_k - w) \cdot n_k + q_k \cdot n_k \rangle^* \) |

\[ \Gamma_s = -\Gamma_I = \Gamma \]  

\[ M_s = -M_I = M \]  

\[ Q_s + Q_I = 0 \]
Constitutive relationship

Mechanical behavior
At the microscopic level, it is generally admitted that the liquid metal behaves like a Newtonian fluid, so it is governed by the classical constitutive equations:

\[ s_{\parallel l} = 2\mu_l \overrightarrow{D}(\nabla_j) \]  

(22)

where \( \mu_l \) is its viscosity and \( \overrightarrow{D}(\nabla_j) \) denotes the deviatoric part of the strain-rate tensor \( \overrightarrow{D}(\nabla_j) = (\nabla\nabla_j + \nabla_j \nabla) \). Taking the average of this equation leads to no simple result. As mentioned in [4], a rather rigorous formulation can be obtained under the assumption of macroscopic isotropy but, in our sense, this would lead to useless numerical complications. For simplicity, as done in [2] and [5], it will be assumed that the macroscopic stress strain-rate relations for the liquid phase is given by

\[ \langle s_{\parallel l} \rangle = 2\mu_l \overrightarrow{D}(\nabla_j) \]  

(23)

Experimental results gained in the study of the behavior of metallic powders at high temperature [7], [8], show that the solid phase in the mushy state is mainly viscous and deforms by power law creep. Its constitutive equations may therefore be represented by the Norton-Hoff law, relating the equivalent stress \( \sigma_{eq} \) to the equivalent strain rate \( D_{eq} \):

\[ \sigma_{eq} = K_s \langle D_{eq} \rangle^m \]  

with

\[ \sigma_{eq}^2 = \frac{3}{2} s_{\parallel s} : s_{\parallel s} \quad \text{and} \quad D_{eq}^2 = \frac{2}{3} \overrightarrow{D}(\nabla_j) : \overrightarrow{D}(\nabla_j) \]  

(24)

(25)

Thus constitutive equations of the solid phase at the microscopic scale is modeled as

\[ s_{\parallel s} = \frac{2}{3} K_s \langle D_{eq} \rangle^{m-1} \overrightarrow{D}(\nabla_j) \]  

(26)

where \( K_s \) (Pa.s\(^m\)) is a function of temperature called consistency, and \( m \) is the power law index, also depending on temperature only.

Figure 2: iso-equivalent stress curves in the \((I_\sigma, \sqrt{J_\sigma})\) plan: \( \sigma_{eq} = 1 \) MPa, \( A = 1 \), different values of \( B \).

Here again, an explicit formulation of the macroscopic behavior by the spatial averaging method is impossible and a phenomenological approach is required. Adopting an approach similar to the one of N’Guyen et al. [13] for the modeling of alloys in the semi-solid state which was inspired by soils mechanics works [10], [11], we adopt a compressible viscoplastic formalism for the modeling of the macroscopic behavior of the solid phase. The state of stress is therefore described by means of eq. (24), but with an equivalent stress \( \sigma_{eq} \) depending on the isotropic part of stresses, as illustrated by Figure 2:
\[ \sigma_{eq}^2 = A(g_s)I_\sigma + B(g_s)I_\sigma^2 \]
with the two first invariants of macroscopic stress tensor defined as
\[ I_\sigma = \left\langle s_{ss} : \delta \right\rangle \quad \text{and} \quad J_\sigma = \left\langle S^s : S^s \right\rangle \]

\( S^s \) being the deviatoric part of \( \left\langle s_{ss} \right\rangle \). The behavior is therefore defined by two rheological functions \( A \) and \( B \) that depend on the volume fraction \( g_s \) and on the interfacial structures. Expressions for those coefficients can be found in [8], [12] or [13] for different materials.

Finally, the macroscopic constitutive relationship of the solid phase takes the explicit form:
\[ \left\langle s_{ss} \right\rangle = K_s D_{eq} m^{-1} \left[ \frac{1}{9B} I_D \delta + \frac{1}{A} \overline{D}(V^s) \right] \]

where \( K_s \) and \( m \) are the intrinsic consistency and power-law index of the solid phase (eq. (26)) and where the equivalent strain-rate associated to \( \sigma_{eq} \) as defined by eq. (27) can be proved to be
\[ D_{eq}^2 = \frac{1}{A} J_D + \frac{1}{9B} I_D^2 \left. , \quad \text{with} \quad I_D = \overline{D}(V^s) : \delta \quad \text{and} \quad J_D = \overline{D}(V^s) : \overline{D}(V^s) \right) \]

**Thermal behavior**

Phases are assumed at local thermal equilibrium, as done in [5]:
\[ T_s = T_l = T \]
This is a classical assumption that was proved to be valid for a macroscopic description if both phases do not exhibit too different thermal properties and if thermal barriers between phases are not too important [9]. Fortunately, it will be the case for most solidification processes. Hence, neglecting the effect of pressure, specific enthalpies of each phase are written as functions of temperature \( T \) only:
\[ h_s = c_p T_s \quad \text{and} \quad h_l = c_p T_l + L^s \rightarrow l \]
where \( L^s \rightarrow l \) denotes the latent heat of fusion and \( c_p \) the heat capacitance. As most practical alloys involve solidification intervals of about a hundred degrees, \( c_p \) is supposed to be constant, which seems a reasonable assumption for the description of the mushy state.

Thanks to the macroscopic isotropy assumption, the average heat flux density of phase \( k \) will be modeled by a simple mixture model as
\[ \langle \dot{q}_{kk} \rangle = -g_k A_k \overline{\nabla T} \]

According to those assumptions, the energy balance may now be rewritten in the form of a single equation, obtained by summing eq. (18) for each phase. Then accounting for eq. (16) and (21), we get the final expression of the energy conservation equation:
\[ \left\langle \rho \right\rangle \frac{\partial H}{\partial t} + \left\langle \rho \dot{\mathbf{V}} \right\rangle : \nabla \mathbf{H} + \nabla : \left\langle \dot{q} \right\rangle = 0 \]

where the following notations were introduced:
\[ H = g_s h^s + g_l h^l = c_p T + f_l L^s \rightarrow l \quad ; \quad \left\langle \rho \right\rangle = g_s \rho^s + g_l \rho^l \]
\[ \left\langle \dot{q} \right\rangle = \left\langle \dot{q}^s \right\rangle + \left\langle \dot{q}^l \right\rangle = -\left( g_s \lambda^s + g_l \lambda^l \right) \overline{\nabla T} \quad ; \quad \left\langle \rho \dot{\mathbf{V}} \right\rangle = \rho^s \dot{\mathbf{V}}^s + \rho^l \dot{\mathbf{V}}^l \]

**Modeling of interfacial exchanges**

The additional source terms arising in macroscopic balance have to be expressed in terms of macroscopic variables \( (V_k, \rho^k, g_k) \). As the spatial averaging method no longer brings further information, phenomenological considerations have to be employed.
Momentum exchange

According to the expression of local constitutive equations (14), the momentum exchange term \( \mathbf{M} \) defined in Table 3 can be parted into:

\[
\mathbf{M} = \mathbf{M}^p + \mathbf{M}^d
\]  

(36)

with

\[
\mathbf{M}^p = -\left(p^s \mathbf{n}_s \right)^* = \left(p^l \mathbf{n}_l \right)^* \quad \text{and} \quad \mathbf{M}^d = \left( \mathbf{s}_s \cdot \mathbf{n}_s \right)^* = -\left( \mathbf{s}_l \cdot \mathbf{n}_l \right)^*
\]  

(37)

Both phases being incompressible, it seems natural to assume that the equilibrium of pressure \( p_k \) is almost instantaneous, so that \( p_k \) equals its average value \( \bar{p} \) and equals its value on the interface. The continuity of pressure at the interface \( A \) thus enables to write

\[
p_s = p^s = p_l = p^l = p
\]  

(38)

A single hydrostatic pressure \( p \) can therefore be defined. Then using averaging theorems we deduce from (37) and (38) that

\[
\mathbf{M}^p = -p \left( \mathbf{n}_s \right)^* = p \nabla g_s = -p \nabla g_l
\]  

(39)

For sufficiently high solid fractions, the momentum exchange due to the deviatoric part of stresses is very often interpreted as the interaction force generated by the flow of the liquid through the solid skeleton, the latter being considered as a rigid porous medium. The liquid phase being assumed Newtonian and the microstructure isotropic, \( \mathbf{M}^d \) can be modeled by a filtration law of the Darcy type, written in terms of the relative velocity [7]:

\[
\mathbf{M}^d = -\frac{\frac{g_l \mu_l}{K(g_s)}}{g_l} \left[ \frac{\mathbf{V}^l - \mathbf{y}^s}{g_s} \right] = -\frac{\frac{g_l \mu_l}{K(g_s)}}{g_l} \left[ \mathbf{V}^l - \frac{g_s}{g_s} \mathbf{V}^s \right]
\]  

(40)

Various different models can be used in order to evaluate the value of permeability \( K \) in terms of the solid fraction and of microstructural parameters.

For lower solid fractions, i.e. below the coherency fraction, the solid phase is mainly made of isolated grains moving through the liquid. Interaction force \( \mathbf{M}^d \) may therefore be modeled by a drag force, as proposed by Ni and Beckerman [4], which can be expressed exactly in the form of eq. (40) with a different expression of the permeability coefficient.

Mass transfer

In the case of a static homogeneous solidification problem, the evolution of the solid volume fraction is directly linked to the evolution of temperature and is calculated by the use of a diagram \( g_s = F(T) \) or \( g_s = F(H) \). According to eq. (16), such a simple approach is not valid anymore in the case of a general two-phase thermo-mechanical problem because the evolution of \( g_s \) also depends on mechanical effects. However, considering a static case of solidification (e.g. \( \mathbf{V}'=0 \)), eq. (16) shows that we have \( \rho_s \frac{\partial g_s}{\partial t} = \Gamma \). \( \Gamma \) can therefore be interpreted as the mass transfer rate due to solidification that would occur in a static situation. As a rough approximation, it will be calculated from function \( F \) as

\[
\Gamma = \rho_s \frac{\partial F}{\partial t}(H) = \rho_s \frac{\partial F}{\partial H}(H) \frac{\partial H}{\partial t}
\]  

(41)

Such an approximation thus enables the calculation of volume fraction evolution by the solving of energy balance equation (34). Nevertheless, according to the works of Wang and Beckermann [6], a more realistic expression should involve a full calculation of species conservation equations in both phases, which is not in the scope of this work.
Table 4: Final balance equations set of the adopted two-phase model.

<table>
<thead>
<tr>
<th>Category</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass (solid)</td>
<td>[ \frac{\partial g_s}{\partial t} + \nabla \cdot \mathbf{v}^s = \frac{\Gamma}{\rho_s} ] (42)</td>
</tr>
<tr>
<td>Mass (solid+liquid)</td>
<td>[ \nabla \cdot \left( \mathbf{v}^s + \mathbf{v}^l \right) = \frac{1}{\rho_s} - \frac{1}{\rho_l} \Gamma ] (43)</td>
</tr>
<tr>
<td>Momentum (solid)</td>
<td>[ \rho_s \frac{\partial \mathbf{v}^s}{\partial t} + \rho_s \nabla \cdot \left( \frac{1}{g_s} \mathbf{V}^s \otimes \mathbf{v}^s \right) = \nabla \cdot \left( \mathbf{s}^s \right) - g_s \nabla p + g_s \rho_s \mathbf{g} + \frac{g_l \mu_l}{K} \left( \mathbf{v}^l - \frac{g_l}{g_s} \mathbf{v}^s \right) ] (44)</td>
</tr>
<tr>
<td>Momentum (liquid)</td>
<td>[ \rho_l \frac{\partial \mathbf{v}^l}{\partial t} + \rho_l \nabla \cdot \left( \frac{1}{g_l} \mathbf{V}^l \otimes \mathbf{v}^l \right) = \nabla \cdot \left( \mathbf{s}^l \right) - g_l \nabla p + g_l \rho_l \mathbf{g} - \frac{g_l \mu_l}{K} \left( \mathbf{v}^l - \frac{g_l}{g_s} \mathbf{v}^s \right) ] (45)</td>
</tr>
<tr>
<td>Energy (solid+liquid)</td>
<td>[ \langle \rho \rangle \frac{\partial H}{\partial t} + \langle \rho \mathbf{v} \rangle \cdot \nabla H + \nabla \cdot \mathbf{q} = 0 ] (46)</td>
</tr>
</tbody>
</table>

Resolution strategy

The two phase thermo-mechanical problem can now be summarized as done in Table 4. Here the global mass conservation (43) was obtained by summing (16) on both phases. In view of the huge number of variables (7 for a 2D problem, 9 for a 3D one) we propose to develop the resolution scheme represented in Figure 3. It is firstly based on a classical weakly coupled mechanical and thermal resolution, the thermal problem being solved in terms of the total enthalpy variable. Additional equation (42) for the determination of the solid fraction, also coupled in a weak form, is solved just after the mechanical problem, taking as data \( \mathbf{v}^s \) and \( \Gamma (H) \).

Nevertheless, the mechanical problem still implies the determination of two velocity fields and one pressure field so a weakly coupled resolution of liquid and solid momentum equations is also envisaged. The liquid momentum balance (45) is first solved together with the global mass balance (43). The formulation obtained is then similar to the one proposed by Rappaz et al. [5], it is similar to a classical Navier-Stokes "velocity+pressure" problem, with an additional "Darcy term" due to the mechanical interaction with the solid phase and additional volume change sources. Taking \( \mathbf{v}^l \) and \( p \) as data, the solid momentum balance is then also solved in the form of a velocity+pressure problem. This is achieved by introducing the variable \( p^v \) (viscous pressure) defined as:

\[ \langle \mathbf{s}^s \rangle = - p^v \delta + \mathbf{S}^s \] (47)

and by imposing an additional equation that ensures that \( p^v \) equals the isotropic part of the solid stress tensor:

\[ 9B \times p^v = -9B \times \frac{1}{3} \text{trace} \left( \mathbf{s}_{ss} \right) = -K_s D_{eq} m^{-1} I_D \] (48)

From a numerical point of view, the choice of solving two similar velocity+pressure problems is important. It should make possible a continuous resolution of solidification problems from the liquid state to the fully solid state, as visible from equations (44) and (45). As clear from equation (48), when the considered material point tends to be solid, coefficient \( B \) tends to 0 and (48) derives in \( I_D = \nabla \cdot \mathbf{v}^s = 0 \), so the solid phase is treated as incompressible and viscoplastic, which is consistent with the modeling assumptions.
Conclusions

The presented thermo-mechanical two-phase model including the solid phase behavior is an original contribution in the field of the study of solidification processes. Up to now, in the literature, the solid phase of the mushy zone has generally been assumed to be fixed or non-deformable what leads to tremendous simplifications of balance equations, but may lead to non-physical predictions. The present model is a first step toward a more rigorous approach, it has now been implemented in a 2D finite element code and first results should be available soon.

Bibliography