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Macroscopic model for solidification in porous media

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A R T I C L E I N F O

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ABSTRACT

A macroscopic model for solidification of pure metal in porous media is derived using the volume averaging method. Solidification starts when the infiltration of the porous mould is completed and therefore the phase change problem involving three phases (liquid and solid metal, mould) is governed by diffusion. The upscaled model is first characterized by the local thermal equilibrium assumption (LTE) between the liquid and the solid metallic phases leading to one energy conservation equation for the equivalent metallic phase. On the other hand, local thermal non-equilibrium (LTNE) between the equivalent continuous metallic phase and the mould is considered, giving rise to two coupled energy conservation equations. The associated closure problems are derived and numerically solved allowing for the determination of the effective transport properties. Numerical solutions of the macroscopic model are qualitatively compared with available experiments.

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1. Introduction

Due to its practical interest solidification modeling of pure or multicomponent mixtures has been the subject of an intense research activity during the last decades [1]. For dendritic solidification, macroscopic models based on upscaling procedures such as the volume averaging method [2], have been developed in order to provide a continuous description of the physics taking into account phenomena at the smaller scales [3–6]. This procedure has been found to be particularly efficient for the derivation of averaged conservation equations and the determination of the associated transport properties (permeability, effective conductivity, dispersion coefficient) [7,8]. Note that similar upscaling approaches have been also considered for liquid-vapor phase change problems (drying processes, etc.) and comparison with solid-liquid phase change modeling has been recently published [9,10]. The industrial context of the present analysis concerns the elaboration of aluminum metal foams which are characterized by very large porosity values (of the order of 80%). These porous structures are obtained after solidification of an infiltrated molten metal in a porous casting mould. A general review concerning different phase change in porous media has been proposed by [11]. More recent theoretical or numerical analysis at the local scale have focused on the influence of the pore geometry or the thermal conductivity of the foam material [12-16]. Few experiments have also been carried out

[17,18]. A theoretical model analytically studied the conditions for assuming local thermal equilibrium conditions [19]. However, to our knowledge very few studies have been devoted to a macroscopic representation of liquid-solid phase change in porous media [20–22] and the derivation of an averaged model for such a problem was still missing.

This is the objective of the present work to derive such a macroscopic model for solidification of a pure molten phase in an homogeneous porous medium. The full treatment of this problem would imply to take into account the infiltration by the molten metal, the displacement of the liquid-air interface and therefore to consider four phases. In this first analysis, the complexity will be reduced by assuming that the casting mould is fully infiltrated by the liquid metal (no solidification during infiltration). Under these circumstances, the solidification is governed by diffusion and involves three phases: the liquid and the solid metal and the mould. A volume averaging procedure is used in order to upscale the local conservation equations. Since the thermo-physical properties of the liquid and solid metallic phases are close, the model is derived under the local thermal equilibrium assumption (LTE) leading to one energy conservation equation for an equivalent metallic phase. On the other hand, due to several order of magnitude between the conductivity of the metal and the sand preform a local thermal non-equilibrium (LTNE) is retained giving rise to two coupled energy conservation equations for the three phases. Associated closure problems are derived and numerically solved allowing for the determination of the effective transport properties. Finally, the relevance of the macroscopic model is illustrated through a

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Nomenclature

A _{ij}	interface area between phases <i>i</i> and <i>j</i> (m^{-2})
c_{pk}	Massic heat capacity of phase k (J kg $^{-1}$)
k_k	thermal conductivity in phase k at the pore scale $(W^{-1} K^{-1})$
Н	Massic enthalpy of the metal quid ou pas $(J kg^{-1})$
h_{m_k}	interfacial species exchange coefficients in phase k (s ⁻¹)
L	macroscopic length scale (m)
l_i	lattice vector
L_{f}	fusion latent heat (J kg $^{-1}$)
ℓ_{β}	pore length scale (m)
r_0	characteristic size of the averaging volume (m)
T_k	temperature in the phase k at the pore scale k (K)
t	time (s)

qualitative comparison with some experiments performed at the CTIF (French research and development center, specialized in metal casting).

2. Local problem

As previously said, the infiltration of the homogeneous mould by a molten liquid phase is assumed to be completed. In other words, the porous mould is saturated by a liquid phase (with no flow) whose volume fraction is initially equal to the porosity of the mould. The solidification process is therefore governed by a diffusion process involving three phases: the liquid metal (β -phase), the solidified metal (γ -phase) and the mould (σ -phase) (see Fig. 1). In addition, the liquid and the solid densities are assumed to be close and the shrinkage due to solidification is assumed to be negligible. Therefore, the local energy conservation equations are given by

$$\frac{\partial}{\partial t} \left(\rho_{\beta} H_{\beta} \right) = \nabla \cdot \left(k_{\beta} \nabla T_{\beta} \right) \text{ in the } \beta \text{ phase}$$
(1)

$$\frac{\partial}{\partial t} \left(\rho_{\gamma} H_{\gamma} \right) = \nabla \cdot \left(k_{\gamma} \nabla T_{\gamma} \right) \text{ in the } \gamma \text{ phase}$$
(2)

$$\frac{\partial}{\partial t} \left(\left(\rho_{\sigma} c_{p\sigma} \right) T_{\sigma} \right) = \nabla \cdot \left(k_{\sigma} \nabla T_{\sigma} \right) \text{ in the } \sigma \text{ phase}$$
(3)

where $H_{\beta} = c_{p\beta}T_{\beta} + L_f$ is the enthalpy of the liquid metal, L_f represents the heat latent and $H_{\gamma} = c_{p\gamma}T_{\gamma}$ is the solid enthalpy. k_i (for



Fig. 1. Schematic representation of the mould with the averaging volume.

\mathbf{w}_{ij}	interfacial velocity at A_{ij} (m s ⁻¹)
Notatio	ons
$\langle \psi_k \rangle$	superficial average of Ψ_k
$\langle \psi_k \rangle^k$	intrinsic average of Ψ_k
$\widetilde{\psi}$	deviation of Ψ_k
Greek s	symbols

 ε_k volume fraction of phase k ρ_k density of phase k (kg m⁻³)

 $i = \beta, \gamma, \sigma$) is the thermal conductivity of phase *i*. The associated boundary conditions are written at the three interfaces locations $A_{\beta\gamma}, A_{\beta\sigma}$, and $A_{\gamma\sigma}$:

$$\mathbf{n}_{\beta\gamma} \cdot \left(k_{\gamma} \nabla T_{\gamma} - k_{\beta} \nabla T_{\beta} \right) = \mathbf{n}_{\beta\gamma} \cdot \mathbf{w}_{\beta\gamma} \left(\rho_{\gamma} H_{\gamma} - \rho_{\beta} H_{\beta} \right) \text{ at } A_{\beta\gamma}$$
(4)

$$T_{\beta} = T_{\gamma} = T_{\text{fusion}} \text{ at } A_{\beta\gamma} \tag{5}$$

$$T_{\gamma} = T_{\sigma} \text{ at } A_{\gamma\sigma} \tag{6}$$

$$\mathbf{n}_{\gamma\sigma} \cdot k_{\gamma} \nabla T_{\gamma} = \mathbf{n}_{\gamma\sigma} \cdot k_{\sigma} \nabla T_{\sigma} \text{ at } A_{\gamma\sigma}$$

$$\tag{7}$$

$$T_{\beta} = T_{\sigma} \text{ at } A_{\beta\sigma} \tag{8}$$

$$\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla T_{\beta} = \mathbf{n}_{\beta\sigma} \cdot k_{\sigma} \nabla T_{\sigma} \text{ at } A_{\beta\sigma}$$
(9)

This local problem is up-scaled in the next section.

3. Up-scaling

The macroscopic conservation equations are derived using a volume averaging procedure [2] whose definitions and theorems are recalled in Appendix A.

3.1. Mass conservation

Due to the solidification process, it is important to consider first the upscaling of the metal mass conservation. For the motionless β phase ($\mathbf{v}_{\beta} = 0$) we have

$$\frac{\langle \partial \rho_{\beta}}{\partial t} \rangle = \frac{\partial}{\partial t} \left(\varepsilon_{\beta} \langle \rho_{\beta} \rangle^{\beta} \right) - \frac{1}{V} \int_{A_{\beta\gamma}} \rho_{\beta} \mathbf{n}_{\beta\gamma} \cdot \mathbf{w}_{\beta\gamma} dA_{\beta\gamma} - \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \rho_{\beta} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} dA_{\beta\sigma}}_{\mathbf{w}_{\beta\sigma} = 0} = 0$$
(10)

Since the mould is rigid, the interfacial phase velocities $\mathbf{w}_{\beta\sigma} = \mathbf{0}$ and Eq. (10) reduces to:

$$\langle \rho_{\beta} \rangle^{\beta} \frac{\partial \varepsilon_{\beta}}{\partial t} = \underbrace{\frac{1}{V} \int_{A_{\beta\gamma}} \rho_{\beta} \mathbf{n}_{\beta\gamma} \cdot \mathbf{w}_{\beta\gamma} dA_{\beta\gamma}}_{\text{Phase change rate}} = \dot{m}_{\beta}$$
(11)

where \dot{m}_{β} is the phase change rate. Similar average for the γ -phase gives:

$$\langle \boldsymbol{\rho}_{\gamma} \rangle^{\gamma} \frac{\partial \boldsymbol{\varepsilon}_{\gamma}}{\partial t} = -\frac{1}{V} \int_{\boldsymbol{A}_{\beta\gamma}} \boldsymbol{\rho}_{\gamma} \, \mathbf{n}_{\beta\gamma} \cdot \mathbf{w}_{\beta\gamma} \, d\boldsymbol{A}_{\beta\gamma} = \dot{\boldsymbol{m}}_{\gamma} \tag{12}$$

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