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Upscaling approach for macroscopic solidification problems

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ABSTRACT

The study presented in this paper arises from the general necessity of developing simulation tools at the scale of industrial processes or natural phenomena to describe coupled mechanisms governing heat and mass transfer and fluid flow in divided media at a much smaller scale. The use of the volume averaging method with closure presented by S. Whitaker [1] has proved to be a very powerful tool for deriving macroscopic models allowing for taking into account local features through the determination of the effective properties by solving the associated local closure problems on specific porous matrix geometries.

One of the most challenging solidification problem is the modeling and simulation of columnar dendritic solidification of binary mixtures – typically metallic alloys – which allows to extend the approach to the interfacial "mushy" zone of a solidifying system. The specificity of the problem concerns several features :

- 1. the porous structure is the growing dendritic phase itself saturated by the liquid phase and evolves in time. The treatment of the solid-liquid interface velocity is still a challenging issue,
- 2. the dendrites are oriented along the temperature gradient which controls the solidification. The porosity is continuously varying from 0 in the growing solid to 1 in the bulk liquid phase, leading to spatially evolving heterogeneities which raise specific problems in the determination of the effective properties [2],
- 3. while the thermal local equilibrium may be assumed in the interfacial region, this is not verified for species conservation and the model has to account for local mass non equilibrium [3].

Due to this complexity, most solidification models were making use of empirical conservation equations and ad hoc constitutive laws. The equations derived from the averaging method and the associated closure problem allowed to identify the different terms and to complete the description of the phenomenon at the macroscopic scale [4]. The limitation of the method in terms of the predictive capacity of the model is that the topology of the local dendritic structure, has to be a priori known to allow for the resolution of the closure problem and for the determination of the effective properties.

The method is also applied to a second kind of solid-liquid phase change problems : the infiltration a porous preform by a pure liquid metal and its subsequent solidification. This process is used in the casting of metallic foams and involves three different phases, the liquid and solid metal and the solid preform.

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