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► To cite this version:

Jean-Christophe Gebelin, Christian Geindreau, Laurent Orgéas, Pascale Royer, Denis Favier, et al.. Influence of the liquid flow through the solid skeleton on the overall deformation of a material in semi-solid state. 6th International Conference on the Semi-Solid Processing of Alloys and Composites , Sep 2000, Turin, Italy. hal-01717372

HAL Id: hal-01717372

<https://hal.science/hal-01717372>

Submitted on 30 Aug 2018

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INFLUENCE OF LIQUID FLOW THROUGH THE SOLID SKELETON ON THE OVERALL DEFORMATION OF METALLIC ALLOYS IN SEMI-SOLID STATE

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ABSTRACT: In order to predict macrosegregation occurring during thixoforming of metallic alloys, an isothermal two-phase model has been implemented in a finite element code. In this model, the solid phase is considered to be a porous viscoplastic continuous medium, and the flow of the liquid phase through the solid skeleton is assumed to verify the well-known Darcy's law. We show that macrosegregation observed during simple compression experiments is well simulated at low strain rates but that the model fails at reproducing these tests at high strain rates. Then, we use a correction of Darcy's law that accounts for inertial drag forces, and that has been derived by an upscaling technique, so as to improve the simulation results at high strain rates.

KEYWORDS: Two-phase modelling, Darcy's law, upscaling method, numerical simulation

1 INTRODUCTION

Semi-solid slurries are usually considered as homogeneous, non-Newtonian, stress and history dependent fluids. However, on the microscopic scale, a semi-solid slurry is a two-phase system that comprises a solid in equilibrium surrounded with its near-Newtonian parent liquid. In that respect, two-phase macroscopic models are increasingly proposed and studied in order to model and analyse deformation of alloys in semi-solid state [1-4]. These models are aimed at predicting the deformation of the solid skeleton and the liquid flow through the solid skeleton, which may lead to macrosegregation during forming processes such as thixoforming or continuous casting that involve alloys in semi-solid state.

Extensive experimental and theoretical studies have been conducted on the modelling of the solid skeleton deformation [1,5,6]. Comparatively, the influence of the liquid flow through the solid skeleton on the overall slurry deformation has not yet been well-studied. Under steady state conditions and with no solid fraction gradient, it is generally proposed that neglecting inertia drag forces, the liquid flow through the solid sponge is governed by Darcy's law. Based on this assumption, numerical simulation of compression tests shows that segregation occurring at low strain rates is well reproduced. However, this model fails at predicting the homogeneity of the semi-solid deformation which is experimentally observed at high strain rates. In this paper, we show that results of simulation are improved if local inertia drag forces are taken into account. This leads to correct the usual Darcy's law by a term which is cubic in the seepage velocity, as it has been proved via an upscaling approach in [7-9]. This term is relevant for non turbulent fluid flow and local Reynolds number up to 100.

In section 2, we briefly summarise the isothermal two-phase formalism which is used in the developed finite element code. Then, section 3 is aimed towards analysing the simulation results obtained when Darcy's law is used for modelling fluid flow. In particular, we show that these results predict a local Reynolds number which is greater than the limit value associated with the use of Darcy's law. Then, section 4 sets out to present a correction of Darcy's law. Simulation of plane compression tests at high strain rates demonstrates the need of such correction for an accurate prediction of macrosegregation.

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2 NUMERICAL MODEL

We have developed an isothermal two-phase finite element code for modelling the behaviour of semi-solid metals during thixoforming [9]. In this code, the description we have adopted is expressed with respect to two independent variables, namely, the particles of the solid skeleton and the time. Our presentation is restricted to a saturated semi-solid medium where there is no phase change. Following the theoretical two-phase framework [10], these hypotheses lead to the following writing of the mass balance equations of the solid phase (s) and the liquid phase (l), respectively [2]:

$$\begin{cases} \frac{D^{(s)}}{Dt} (\rho_{(s)} f^{(s)}) + f^{(s)} \rho_{(s)} \operatorname{div} \tilde{v}^{(s)} = 0 \\ \frac{D^{(l)}}{Dt} (\rho_{(l)} (1 - f^{(s)})) + (1 - f^{(s)}) \rho_{(l)} \operatorname{div} \tilde{v}^{(l)} = 0 \end{cases} \quad (1)$$

where $f^{(s)}$ is the solid volume fraction, $\rho_{(\alpha)}$ and $\tilde{v}^{(\alpha)}$ are the intrinsic density and the velocity field of the α -phase, and $\frac{D^{(\alpha)}}{Dt}$ is the material time-derivative following an α -particle, respectively.

Assuming that inertial effects are negligible and that there is no external volume forces, the first momentum balance equations for the solid-phase (s) and the liquid-phase (l) are respectively given by:

$$\begin{cases} -f^{(s)} \operatorname{grad} p_i + \operatorname{div} \hat{\sigma}_{\approx}^{(s)} - \pi_{\approx}^{(s/l)} = 0 \\ -(1 - f^{(s)}) \operatorname{grad} p_i + \pi_{\approx}^{(s/l)} = 0 \end{cases} \quad (2)$$

where p_i , $\hat{\sigma}_{\approx}^{(s)}$ and $\pi_{\approx}^{(s/l)}$ are the interstitial pressure, the effective stress tensor of the solid phase, and the solid-liquid momentum exchange, respectively. Eq.(2)b implies that the partial liquid stress is supposed to be purely hydrostatic [2]. It is further assumed that the solid skeleton is an isotropic, purely viscoplastic and compressible medium. Introducing, as in [1,5,9], the Abouaf's equivalent stress $\hat{\sigma}_{eq}^{(s)}$ yields :

$$\hat{\sigma}_{eq}^{(s)2} = A(f^{(s)}) \operatorname{tr}^2 \hat{\sigma}_{\approx}^{(s)} + B(f^{(s)}) \left[\hat{\sigma}_{\approx}^{(s)} - \frac{1}{3} \operatorname{tr} \hat{\sigma}_{\approx}^{(s)} \delta_{\approx} \right] : \left[\hat{\sigma}_{\approx}^{(s)} - \frac{1}{3} \operatorname{tr} \hat{\sigma}_{\approx}^{(s)} \delta_{\approx} \right] \quad (3)$$

the solid phase strain rate tensor $D_{\approx}^{(s)}$ is then determined using the following constitutive relationships:

$$D_{\approx}^{(s)} = \frac{1}{2} \left(\operatorname{grad} \tilde{v}^{(s)} + {}^T \operatorname{grad} \tilde{v}^{(s)} \right) = \beta e^{\frac{Q}{RT}} \hat{\sigma}_{eq}^{(s)n} \frac{\partial \hat{\sigma}_{eq}^{(s)}}{\partial \hat{\sigma}_{\approx}^{(s)}} \quad (4)$$

where A and B are rheological functions and n , β , Q are constitutive parameters.

The solid-liquid momentum exchange is usually such that under isothermal steady-state conditions and when there is no solid deformation, the momentum balance equation (2)b reduces to the well-known Darcy's law. This implies:

$$\pi_{\approx}^{(s/l)} = - \frac{(1 - f^{(s)}) \mu_{(l)}}{K} (\tilde{v}^{(l)} - \tilde{v}^{(s)}) = - \frac{(1 - f^{(s)}) \mu_{(l)}}{K} \tilde{v}^{(r)} \quad (5)$$

In this latter equation, $\tilde{v}^{(r)}$ is the relative velocity field, $\mu_{(l)}$ is the Newtonian viscosity of the liquid phase and K is the permeability of the solid skeleton. As in [12], K is expressed with respect to the mean solid particle diameter d , and to the volume solid fraction :

$$K = \frac{(1 - f^{(s)})^{\lambda-1} d}{b} \quad (6)$$

where b and λ depend on the microstructure of the solid skeleton.

3 NUMERICAL RESULTS WHEN USING DARCY'S LAW

In order to illustrate the response of such a two-phase model, we considered the rather simple problem of isothermal plane compression of a parallelepiped rectangular semi-solid sample of 40mm width. The simulation is performed using physical data, constitutive parameters and rheological functions of a Sn15%Pb alloy, within the solid fraction range of 0.7-0.9 [13]. They are listed in table 1.

$\rho(l)$	$\mu(l)$	D	λ	B
8100 kg m ⁻³	1 mPa s	100 μm	3	1000
n	β	Q	A	B
5.7	1.54 10 ⁸ MPa ⁻ⁿ s ⁻¹	132 kJ mol ⁻¹	3 $f^{(s)-15}$	0.35($f^{(s)-12} - 1$)

Table 1: Physical data, constitutive parameters, and rheological functions used to run the simulation.

The height of the sample is in the y -direction of compression and the thickness is in the z -direction of the plane strain. Due to symmetry, only half of the width in the x -direction is considered. The simulations show that when neglecting friction during plane compression the results are homogeneous throughout the whole height and the whole thickness of the sample. As a result, only a rectangular parallelepiped of 20x1x1 mm³ is meshed using 1x1x1 mm³ linear hexahedrals. Accordingly to the condition of plane deformation ($\forall M, t \ D_{zz}^{(s)} = D_{zz}^{(l)} = 0$), and to the symmetry of boundary-conditions, a uniform vertical strain rate is applied to the sample, *i.e.* $\forall M, t \ D_{yy}^{(s)} = D_{yy}^{(l)} = D$. D is taken in the range 10⁻³-10³ s⁻¹ which includes the strain rate states encountered during thixotropy. Moreover, at the free surface of the sample, the interstitial pressure is set to zero. At last, we consider the following initial conditions for the simulation: no interstitial pressure ($\forall M$) and initial homogeneous solid fraction $f_o^{(s)}$.

In order to characterise the macrosegregation, a local segregation rate defined as $D_{seg} = \dot{f}^{(s)} / D$ is introduced. Fig. 1(a) show seven evolutions of local segregation D_{seg} , along the sample width when using the usual Darcy-like solid-liquid momentum exchange (eq. (5)). These evolutions are obtained for seven distinct imposed strain rates D , *i.e.* 10⁻³ s⁻¹, 10⁻² s⁻¹, 10⁻¹ s⁻¹, 10⁰ s⁻¹, 10¹ s⁻¹, 10² s⁻¹ and 10³ s⁻¹ and for two initial solid fractions, *i.e.* $f_o^{(s)} = 0.7$ (Fig. 1(a)(I)) and $f_o^{(s)} = 0.9$ (Fig. 1(a)(II)).

A first set of interesting qualitative tendencies are deduced from this figure:

- ✓ Whatever the initial solid fraction is, liquid expulsion is higher at low imposed strain rates. Conversely, samples deformed at high strain rates tend to behave like a one-phase medium: for example, when $f_o^{(s)} = 0.7$ and $D = 10^3$ s⁻¹, no segregation occurs for $x < 14$ mm (Fig. 1(a)(I)). This is precisely what is predicted by the criterion established by an upscaling technique in a previous work [14]. Moreover, it is qualitatively in good accordance with compression experiments performed on semi-solid alloys [15,17]. However, “experimental transition” between two-phase and one phase behaviour for globular semi-solid usually occurs between 10⁰ and 10¹ s⁻¹[15,17]: in the present simulation, such a transition is observed between 10² and 10³ s⁻¹.
- ✓ An increase of the initial solid fraction $f_o^{(s)}$ enhances these tendencies. On the one hand, at low strain rates, the higher the initial solid fraction, the higher the liquid expulsion. The form of the solid viscoplastic model (eq. (3) and (4)) is responsible of such a trend. On the other hand, at high strain rates, an increase of the initial solid fraction leads to an increase of the single-phase behaviour: for example,

when $f_o^{(s)} = 0.9$ and $D = 10^3 \text{ s}^{-1}$, no segregation occurs for $x < 17 \text{ mm}$ (Fig. 1(a)(II)). This is mainly due to the decrease of the solid permeability K which is a function of the solid volume fraction.

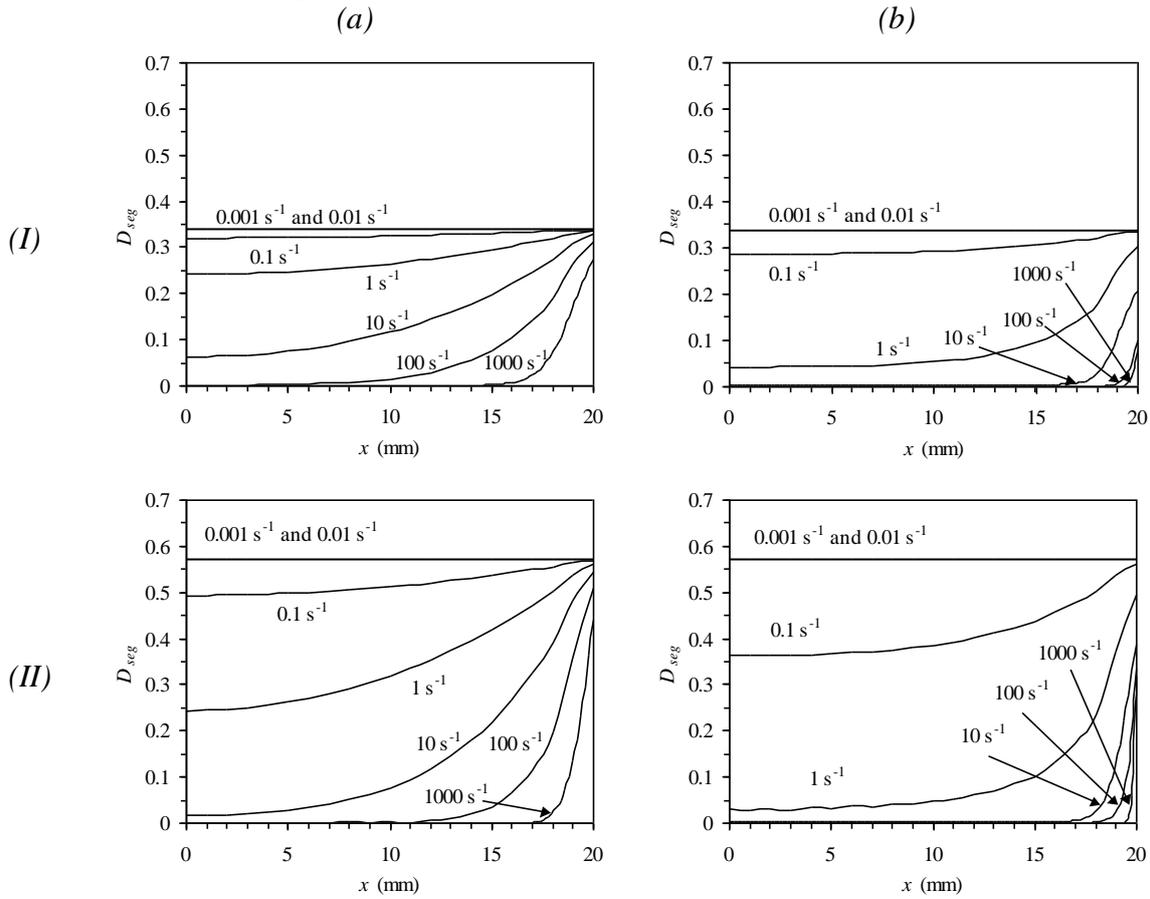


Fig. 1 : Plane compression simulation : segregation rate D_{seg} with respect to the x coordinate at different imposed strain rates D , for $f_o^{(s)} = 0.7$ (I) and $f_o^{(s)} = 0.9$ (II), and for usual solid-liquid momentum exchange, i.e. $\Gamma_D = 0$ (a) and for modified usual solid-liquid momentum exchange, i.e. $\Gamma_D = 10^4$ (b).

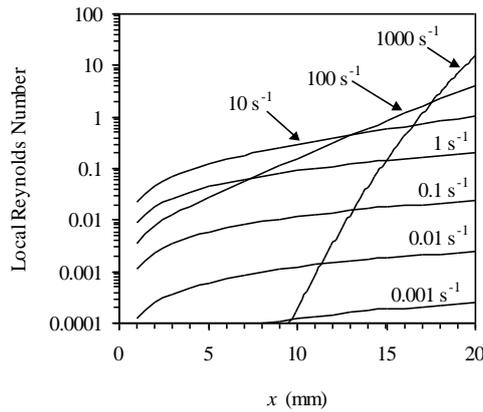


Fig. 2 : Plane compression simulation, $f_o^{(s)} = 0.7$: local Reynolds number with respect to the x coordinate at different imposed strain rates D .

A further analysis can be performed with the help of Fig. 2 in which the evolution of the local Reynolds number Re_{local} , defined by eq. (7) is displayed, for the numerical experiments given in Fig. 1(a)(I).

$$R_{elocal} = \frac{\rho_{(l)} \sqrt{K}}{\mu_{(l)}} \sqrt{\underset{\sim}{v}^{(r)} \cdot \underset{\sim}{v}^{(r)}} \quad (7)$$

where $\rho_{(l)}$ is the intrinsic specific mass of the liquid phase. Predicted modified local Reynolds number higher than 10^{-1} are observed for $D > 10^0 \text{ s}^{-1}$. In that case, a usual solid-liquid momentum exchange as defined by eq. (5) becomes irrelevant and thus leads to erroneous results [7]. As shown in the next section, a more realistic model will be proposed to improve the simulation.

4 IMPROVEMENT OF THE LIQUID FLOW

It is generally admitted that for sufficiently low local Reynolds numbers (typically $R_{elocal} \ll 1$), the steady state flow of incompressible Newtonian fluid through porous media is ruled by Darcy's law. As R_{elocal} increases, the flow through porous media becomes non-linear as a result of inertial drag forces. To account for this effect at low but not completely negligible local Reynolds number, *i.e.* $R_{elocal} < 10$, Darcy's law is usually replaced by Forchheimer's equation [18], also known as Ergun's equation [19]. This implies:

$$\underset{\sim}{\pi}^{(s/l)} = -(1-f^{(s)}) \left[\frac{\mu_{(l)}}{K} + \frac{\varphi \rho_{(l)}}{\sqrt{K}} \sqrt{\underset{\sim}{v}^{(r)} \cdot \underset{\sim}{v}^{(r)}} \right] \underset{\sim}{v}^{(r)} \quad (8)$$

Where φ is a constitutive parameter. However, eq.(8) was found to be irrelevant [7] by upscaling fluid flow equations at the pore scale while assuming a periodic isotropic porous medium. Instead, another equation was proposed and was successfully fitted with filtration experiments [8]. Following these recent results, a new solid-liquid momentum exchange has been implemented in the FEM code:

$$\begin{aligned} \underset{\sim}{\pi}^{(s/l)} &= -(1-f^{(s)}) \left[\frac{\mu_{(l)}}{K} + \Gamma_D \frac{\rho_{(l)}^2}{\mu_{(l)}} \underset{\sim}{v}^{(r)} \cdot \underset{\sim}{v}^{(r)} \right] \underset{\sim}{v}^{(r)} \\ &= -(1-f^{(s)}) \frac{\mu_{(l)}}{K} \left[1 + \Gamma_D R_{elocal}^2 \right] \underset{\sim}{v}^{(r)} \end{aligned} \quad (9)$$

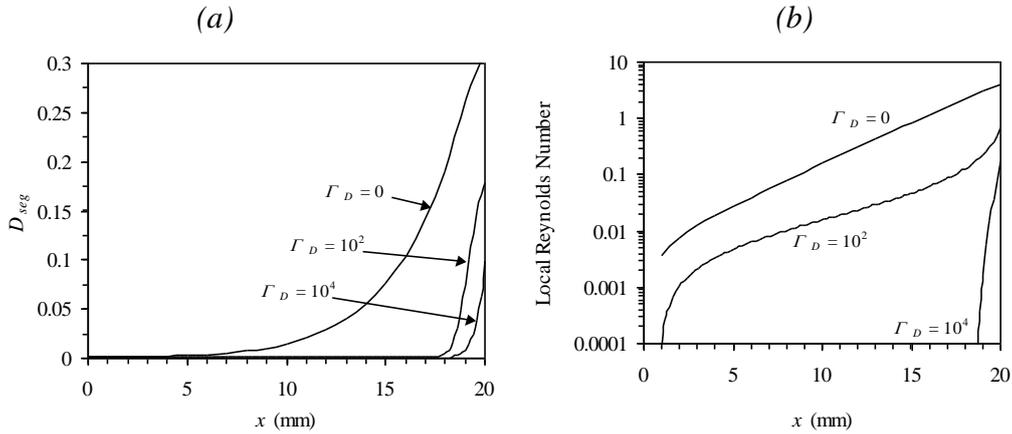


Fig. 3 : Plane compression simulation, $D = 100 \text{ s}^{-1}$, $f_o^{(s)} = 0.7$: Influence of Γ_D on the segregation rate D_{seg} (a) and on the local Reynolds number R_{elocal} (b).

where Γ_D is a dimensionless constitutive parameter. Its influence on the fluid flow through the solid skeleton was explored in the example of Fig. 3. In this figure, the results deduced from a compression plane simulation where $D = 100 \text{ s}^{-1}$ and $f_o^{(s)} = 0.70$, and where Γ_D took respective values of 0, 10^2 and 10^4 are displayed. As shown in Fig. 3(a), an increase of Γ_D leads to a decrease of the predicted liquid expulsion. As a consequence, the predicted local Reynolds number, and hence the relative velocity (see eq. (7)) are decreasing functions of Γ_D (see Fig. 3(b)). It is worth noting that calculated R_{elocal} are consistent with the assumptions used to establish eq. (9), *i.e.* $R_{elocal} < 10$: this is not the case with eq. (5), for which $R_{elocal} \ll 1$.

For qualitatively fitting compression experiments performed on globular semi-solid samples, Γ_D is set to a value which is able to reproduce a two-phase to single-phase behaviour in the strain rate region 10^0 - 10^2 s⁻¹, i.e. $\Gamma_D = 10^4$. Results sketched in Fig. 1(b) show the improvement brought by the new model.

6 CONCLUSION

In this work, a two-phase model has been implemented in a finite element code to predict segregation occurring during thixoforming. To describe the deformation of the solid skeleton, a rather simple isotropic viscoplastic compressible model has been used. The liquid flow through the solid skeleton has initially been described using a classical Darcy-like solid-liquid momentum exchange. The two-phase model succeeded in predicting the segregation observed during deformation of semi-solid alloys at low strain rates. Nevertheless, at high strain rates, the segregation was overestimated and unrealistic fluid velocity fields were obtained. The local Reynolds number has been found to range in a zone where the classical solid-liquid momentum exchange is no longer relevant.

A more physical description of fluid flow through the solid porous medium has then been utilised, which accounts for weak inertial drag forces associated with the liquid phase flow. In that respect, the solid-liquid momentum exchange has been modified, based on previous upscaling works [7-9]. The new fluid flow model requires a dimensionless parameter. Its influence on the semi-solid behaviour has been analysed, and its value has qualitatively been determined to match the experimental observations.

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