



# A mesoscale granular model for the mechanical behavior of alloys during solidification

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## Abstract

We present a two-dimensional granular model for the mechanical behavior of an ensemble of globular grains during solidification. The grain structure is produced by a Voronoi tessellation based on an array of predefined nuclei. We consider the fluid flow caused by grain movement and solidification shrinkage in the network of channels that is formed by the faces of the grains in the tessellation. We develop the governing equations for the flow rate and pressure drop across each channel when the grains are allowed to move, and we then assemble the equations into a global expression that conserves mass and force in the system. We show that the formulation is consistent with dissipative formulations of non-equilibrium thermodynamics. Several example problems are presented to illustrate the effect of tensile strains and the availability of liquid to feed the deforming microstructure. For solid fractions below  $g_s = 0.97$ , we find that the fluid is able to feed the deformation at low strain, even if external feeding is not permitted. For solid fractions above  $g_s = 0.97$ , clusters of grains with “dry” boundaries form and fluid flow becomes highly localized.

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## 1. Introduction

The last-stage solidification of alloys is a critical step in casting and welding processes during which several defects can form [1]. In addition to porosity, the most severe of these defects is probably hot cracking, *i.e.* a spontaneous failure of the material while it is still semi-solid. This defect, which typically occurs in dilute and hard alloys, limits the productivity of cast houses and restricts the range of alloys that can be produced [2]. It also severely limits the weldability of this class of alloys.

In dilute alloys, solid grains are separated by thin continuous liquid films up to high volume fraction of solid  $g_s$

(typically up to  $g_s \approx 0.95$ ), especially at high-angle grain boundaries, where coalescence of solid grains is made difficult by the large grain boundary energy [3]. As stresses and strains are generated in the not yet fully coherent solid, the presence of these liquid films together with the low permeability of the mushy zone near  $g_s = 0.95$ , which prevents efficient feeding, makes the material extremely brittle [4,5]. Deformation induced by thermal and solidification shrinkage tends to localize at these liquid films, which act as a brittle phase. They pose little resistance to tensile strains and, as they open, the newly created volume cannot be fed by intergranular liquid. The so-called “brittle range”, meaning the  $g_s$  range where the mushy zone exhibits low strength and low ductility, can be measured, for example, by tensile tests on partially solidified alloys [6–8].

Accurate prediction of hot cracking requires the knowledge of:

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retains the main physical aspects at the scale of the grains yet is simple enough to be computationally tractable. To that end, the following assumptions are made:

- (1) *The grains are undeformable.* This assumption is adequate to obtain insight into the physics of hot tearing, where deformations are small. A more complete model of the rheology of the mushy zone should also include deformation of the solid, which is known to be important for volume fractions of solid  $g_s \gtrsim 0.6$ , known as the traction coherency solid fraction [7,28,29].
- (2) *Grain movement can occur only by translation.* This hypothesis seems very restrictive, but experimental studies have shown that at high temperature and high solid fraction the most important deformation mechanism is grain boundary sliding [6]. Making this assumption greatly improves the computational efficiency of the model, because detection of contacts between polygonal grains is difficult if rotations are permitted [20].
- (3) *Liquid channels smaller than a predefined coalescence interaction distance  $\delta$ , on the order of a few nanometers, are taken to be fully solid [23,3].* Using such a cut-off improves the computational behavior of the model by eliminating very large coefficients that would otherwise appear in the matrix of the linear system derived in Section 3.5.
- (4) *The intergranular fluid is Newtonian and incompressible, and no-slip conditions apply at the solid–liquid ( $s - \ell$ ) interface.* We adopt this constitutive model for the fluid even though the channels between grains are very thin. We note that measurements by Israelachvili [30] and Tabeling [30,31] showed that the viscosity observed in bulk samples is still valid for films as thin as 5 nm. Another effect observed in thin films is slipping at  $s - \ell$  interfaces, which may be due to the formation of a nanometer scale air gap [32,31]. This phenomenon occurs when the shear stress exceeds a critical value, and might be an interesting phenomenon to consider in hot tearing, especially if gas porosity appears at grain boundaries. It is not included in this work.

### 3.2. Notation

Our model considers the liquid network formed between the grains. The basic element is a liquid channel surrounded by two solid grains, designated  $a$  and  $b$  in Fig. 1. The element has four integration points. The first two points are the grain centers, denoted  $O_a$  and  $O_b$  for grains  $a$  and  $b$ , respectively. At these points, we consider two conjugate vector quantities, the velocity of the grain  $\{\mathbf{V}\}_{O_a}$  (or  $\{\mathbf{V}\}_{O_b}$ ) and the force exerted by the grain on a liquid channel  $\{\mathbf{F}\}_a$  (or  $\{\mathbf{F}\}_b$ ). The two other integration points are the ends of the liquid channel, denoted  $i$  and  $j$ . The conjugate quantities considered at these points are the fluid flux  $\Phi_i$  (or  $\Phi_j$ ) and the pressure  $P_i$  (or  $P_j$ ). Upper-

case letters are used for these entities at the integration points, whereas lowercase letters are used for the associated fields (e.g.  $\{v\}$  for the velocity and  $p$  for the pressure at any point in the liquid channel).

Relative translation between neighboring grains can produce a mismatch at the extremities of the channel. With reference to Fig. 1, we introduce the following length measures:  $L$  is the length of the  $s - \ell$  interface for one channel,  $L_c$  is the length of the channel where the two grains effectively face each other and  $L_{ja}$  is the length of the  $s - \ell$  interface from the center of the channel to the extremity of grain  $a$  near vertex  $j$ . We also define  $L_{ia} = L - L_{ja}$ . The half-width of the channel is designated as  $h$ . Note also that, even though the channel can be curved at its extremities, it is modeled with straight lines for the calculation of the pressure field.<sup>1</sup> The special case where relative motion of the grains causes their faces to no longer align anywhere *i.e.*,  $L_c = 0$ , is treated in Section 3.6.

The volume change associated with solidification shrinkage *i.e.*, due to the density difference ( $\rho_s - \rho_l$ ) between the solid and liquid phases, produces a compensating flow in the liquid near the interface. It is most convenient to develop the expressions for the flow in terms of the normal and tangential components of the velocity, denoted with superscripts “ $n$ ” and “ $t$ ”, respectively

$$\{\mathbf{V}\}_a = \begin{pmatrix} V_a^t \\ V_a^n \end{pmatrix} = \begin{pmatrix} V_{O_a}^t \\ V_{O_a}^n - \beta v^* \end{pmatrix} \quad (1)$$

where  $\beta$  is the solidification shrinkage ( $\beta = \rho_s/\rho_l - 1$ ), and  $v^*$  is the speed of the  $s - \ell$  interface as given by the solidification model. We choose the element normal vector  $\{\mathbf{n}\}$  to point toward the liquid from grain  $a$ , and the tangential vector  $\{\mathbf{t}\}$  is directed from vertex  $i$  to vertex  $j$ . Note that, due to this orientation convention, the fluid velocity at the interface with grain  $b$  is written as:

$$\{\mathbf{V}\}_b = \begin{pmatrix} V_{O_b}^t \\ V_{O_b}^n + \beta v^* \end{pmatrix} \quad (2)$$

Symmetry of the solidification model implies that the velocity  $v^*$  of the  $s - \ell$  interface of grain  $b$  is equal to that of its neighbor grain  $a$ . The coordinates in the  $\{\mathbf{t}\}$  and  $\{\mathbf{n}\}$  directions are noted  $X$  and  $Y$ , respectively. The origin is defined at the center of the channel (see Fig. 1).

### 3.3. Integration of the constitutive equations

The scaling analysis given in Appendix A shows that the  $X$ -direction momentum balance in the channel reduces to the following simpler relation between the pressure in the liquid channel  $p(X)$  and the fluid velocity:

<sup>1</sup> Note that the flux balances that we introduce in the next section with the polyhedral envelope of the grains are strictly the same as those done for the rounded grains. Indeed, as the fluid will be considered as incompressible, the mass of fluid in between the grains and their polyhedral envelope remains constant.

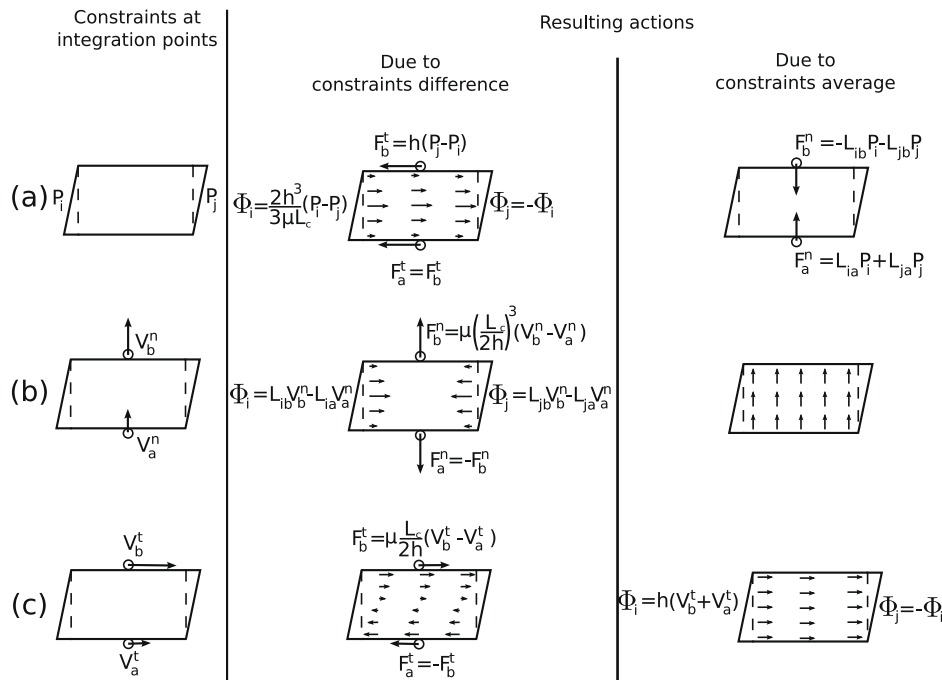


Fig. 2. Representation of the various individual constraints imposed on a liquid channel and on the grains: (a) simple flow in between two immobile grains; (b) normal displacement of the grains; (c) tangential displacement of the grains.

$$\frac{\partial p}{\partial X} = \mu \frac{\partial^2 v_X}{\partial Y^2} \quad (3)$$

where  $\mu$  is the dynamic viscosity. The volumetric flow rate in the channel  $\phi_{i \rightarrow j}(X)$  from vertex  $i$  to vertex  $j$  is defined by

$$\phi_{i \rightarrow j}(X) = \int_{-h}^h v_X(X, Y) dY \quad (4)$$

We also have the continuity equation for a constant density fluid in two dimensions,

$$\frac{\partial v_X}{\partial X} + \frac{\partial v_Y}{\partial Y} = 0 \quad (5)$$

Integrating Eq. 5 over the width of the channel and using the definition of  $\phi_{i \rightarrow j}$  in Eq. (4) gives

$$\frac{\partial \phi_{i \rightarrow j}}{\partial X} = -V^n \quad (6)$$

where

$$V^n = V_b^n - V_a^n = V_{O_b}^n - V_{O_a}^n + 2\beta v^* \quad (7)$$

represents a source or sink in the channel. Note that if the velocity of the grains is zero (or uniform) *i.e.*,  $V^n = 2\beta v^*$ , Eqs. (3) and (6) reduce to those given in Ref. [24], where we considered only the shrinkage-induced intergranular flow.

Eqs. (3) and (6) are integrated in Appendix B for the general case. To provide a better understanding of the underlying physics, let us consider a few special cases where the grain and/or liquid movement isolates the individual contributions of certain important phenomena. Since the governing equations are linear, solutions for cases that

combine these phenomena can be obtained by superposition of these simple cases. The cases are illustrated in Fig. 2.

Case (a), corresponding to the top line of Fig. 2, neglects shrinkage-induced flow ( $\rho_s = \rho_l$ ) and considers an imposed pressure differential between vertices  $i$  and  $j$ . The grain velocities are set to zero for this case. In the part of the channel where the two  $s-l$  interfaces face each other, the fluid velocity profile  $v_X(Y)$  has the usual parabolic profile given by

$$v_X(X, Y) = \frac{1}{2\mu} \frac{\partial p}{\partial X} (Y^2 - h^2) = \frac{P_i - P_j}{2\mu L_c} \frac{\partial p}{\partial X} (Y^2 - h^2) \quad (8)$$

Thus, the volumetric flow rate at the vertices  $i$  and  $j$  is given by:

$$\Phi_i(P_i, P_j) = \frac{2h^3}{3\mu L_c} (P_i - P_j) = -\Phi_j(P_i, P_j) \quad (9)$$

This equation describes the flow between two parallel planes. In two dimensions, any contact between neighboring grains blocks all flow in the channel, whereas in three dimensions the liquid can flow around the contact. To include this important 3-D feature in our 2-D model, we assume that, when two grains make contact, a small “pipe” remains open. The radius of this pipe,  $r_p$ , is estimated to be of the same order of magnitude as the radius of curvature at the grain corner, derived in Ref. [24] (see Fig. 1). Moreover, if the solidification microstructure were to be extended in the third dimension, there would be one such pipe with an average grain diameter  $D_{av}$ . Summing the flow rates for the channel and the pipe gives

$$\Phi_i(P_i, P_j) = \left( \frac{2h^3}{3\mu L_c} + \frac{\pi r_p^4}{8\mu D_{av} L_c} \right) (P_i - P_j) = -\Phi_j(P_i, P_j) \quad (10)$$

where we have represented the flow rate in the pipe using the standard Poiseuille solution.

We show in Appendix A that the pressure loss in the part of the channel where the  $s - \ell$  interfaces of the two grains do not face each other can be neglected with respect to the remaining terms. Therefore, the pressure is constant in these locations, and decreases linearly from  $P_i$  to  $P_j$  along  $L_c$ . This simple pressure profile in the liquid channel can be integrated to obtain the forces exerted by the grains on the liquid to yield

$$\{\mathbf{F}\}_a(P_i, P_j) = \begin{pmatrix} (P_j - P_i)h \\ P_i L_{ia} + P_j L_{ja} \end{pmatrix} \quad (11)$$

and

$$\{\mathbf{F}\}_b(P_i, P_j) = \begin{pmatrix} (P_j - P_i)h \\ -P_i L_{ib} - P_j L_{jb} \end{pmatrix} \quad (12)$$

Of course, the opposite force is exerted by the fluid on the grains.

Next, we consider the individual effect of a grain displacement in the normal direction, with  $V_{O_a}^t = V_{O_b}^t = 0$  and  $P_i = P_j = 0$  (Fig. 2, case (b)). Eqs. (3) and (4), combined with a no-slip condition at the  $s - \ell$  interfaces, link the pressure gradient in the  $X$ -direction to the fluid flow.

$$\Phi_{i \rightarrow j}(X) = -\frac{2}{3\mu} \frac{\partial p}{\partial X} h^3 \quad (13)$$

With the help of Eq. (6), we have then:

$$\frac{2h^3}{3\mu} \frac{\partial^2 p}{\partial X^2} = V_b^n - V_a^n \quad (14)$$

Integrating Eq. (14) twice in  $X$  and considering the imposed symmetry on the pressure gives

$$p(V_a^n, V_b^n) = \frac{3\mu(V_b^n - V_a^n)}{4h^3} \left[ X^2 - \left( \frac{L_c}{2h} \right)^2 \right] \quad (15)$$

This term represents the change in pressure induced by the fluid flow required to compensate the channel expansion ( $V_b^n > V_a^n$ ) or constriction ( $V_b^n < V_a^n$ ). Eq. (15) can be integrated once more over the length of the channel to obtain the forces exerted by the grains on the liquid:

$$\{\mathbf{F}\}_a(V_a^n, V_b^n) = \begin{pmatrix} 0 \\ -\mu(L_c/2h)^3(V_b^n - V_a^n) \end{pmatrix} \quad (16)$$

and

$$\{\mathbf{F}\}_b(V_a^n, V_b^n) = \begin{pmatrix} 0 \\ \mu(L_c/2h)^3(V_b^n - V_a^n) \end{pmatrix} \quad (17)$$

The symmetry of the formulation implies that at the center of the channel

$$\phi_{i \rightarrow j}|_{X=0}(V_a^n, V_b^n) = 0 \quad (18)$$

As the fluid is incompressible, a flux balance is readily written at the channel vertices as

$$\Phi_i(V_a^n, V_b^n) = L_{ib}V_b^n - L_{ia}V_a^n \quad (19)$$

$$\Phi_j(V_a^n, V_b^n) = L_{jb}V_b^n - L_{ja}V_a^n \quad (20)$$

The final case that we consider isolates the effect of tangential displacement of the grains (Fig. 2, case(c)). This situation corresponds to pure shear of the liquid channel, and thus we have:

$$\{\mathbf{F}\}_a(V_a^t, V_b^t) = \begin{pmatrix} -\mu(L_c/2h)(V_b^t - V_a^t) \\ 0 \end{pmatrix} \quad (21)$$

and

$$\{\mathbf{F}\}_b(V_a^t, V_b^t) = \begin{pmatrix} \mu(L_c/2h)(V_b^t - V_a^t) \\ 0 \end{pmatrix} \quad (22)$$

Note that we have neglected the shear forces in the portions of the channel where the two grains do not face each other. Considering the flow relative to the initial (reference) configuration, the average tangential displacement of the grains induces a fluid flow at each vertex given by

$$\Phi_i(V_a^t, V_b^t) = 2h \frac{V_b^t + V_a^t}{2} \quad (23)$$

$$\Phi_j(V_a^t, V_b^t) = -2h \frac{V_b^t + V_a^t}{2} \quad (24)$$

If  $V_a^t = -V_b^t$ , there is no net flow in the channel *i.e.*, the liquid experiences a perfectly symmetric shear stress.

For a more general situation in which all three of the phenomena just discussed may occur, the various contributions to the fluid flow and to the forces on the grains can be written as the sum of the individual simple cases with the result

$$\{\mathbf{F}\}_a = \begin{pmatrix} (P_j - P_i)h - \mu(L_c/2h)(V_b^t - V_a^t) \\ -\mu(L_c/2h)^3 V^n + P_i L_{ia} + P_j L_{ja} \end{pmatrix} \quad (25)$$

$$\{\mathbf{F}\}_b = \begin{pmatrix} (P_j - P_i)h + \mu(L_c/2h)(V_b^t - V_a^t) \\ \mu(L_c/2h)^3 V^n - P_i L_{ib} - P_j L_{jb} \end{pmatrix} \quad (26)$$

$$\Phi_i = \left( \frac{2h^3}{3\mu L_c} + \frac{\pi r_p^4}{8\mu D_{av} L_c} \right) (P_i - P_j) + 2h \frac{V_b^t + V_a^t}{2} + L_{ib}V_b^n - L_{ia}V_a^n \quad (27)$$

$$\Phi_j = \left( \frac{2h^3}{3\mu L_c} + \frac{\pi r_p^4}{8\mu D_{av} L_c} \right) (P_j - P_i) - 2h \frac{V_b^t + V_a^t}{2} + L_{jb}V_b^n - L_{ja}V_a^n \quad (28)$$

We now proceed to develop these expressions into a form suitable for a finite element formulation.

### 3.4. Elementary matrix

In order to obtain a matrix form, we collect the primitive variables into a vector  $\{\mathbf{U}\}^T = (P_i, P_j, V_a^n, V_b^n, V_a^t, V_b^t)$  with the associated flow rates and forces into a second vector  $\{\mathbf{W}\}^T = (\Phi_i, \Phi_j, F_a^n, F_b^n, F_a^t, F_b^t)$ . The superscript “ $T$ ” indicates the transpose of the vector. Eqs. (25)–(28) can then be written in matrix form as

$$\{\mathbf{W}\} = \begin{pmatrix} \Phi_i \\ \Phi_j \\ F_a^n \\ F_b^n \\ F_a^t \\ F_b^t \end{pmatrix} = [\mathbf{E}]\{\mathbf{U}\} = \begin{pmatrix} +C_1 & -C_1 & -L_{ia} & +L_{ib} & +h & +h \\ -C_1 & +C_1 & -L_{ja} & +L_{jb} & -h & -h \\ +L_{ia} & +L_{ja} & +C_2 & -C_2 & 0 & 0 \\ -L_{ib} & -L_{jb} & -C_2 & +C_2 & 0 & 0 \\ -h & +h & 0 & 0 & +C_3 & -C_3 \\ -h & +h & 0 & 0 & -C_3 & +C_3 \end{pmatrix} \begin{pmatrix} P_i \\ P_j \\ V_a^n \\ V_b^n \\ V_a^t \\ V_b^t \end{pmatrix} \quad (29)$$

where

$$C_1 = \left( \frac{2h^3}{3\mu L_c} + \frac{\pi r_p^4}{8\mu D_{av} L_c} \right); \quad C_2 = \mu \left( \frac{L_c}{2h} \right)^3; \quad C_3 = \mu \frac{L_c}{2h} \quad (30)$$

Note that, unlike the usual formulation of mechanical problems using the finite element method, we have chosen to group together the normal and tangential components of the forces and velocities acting on grains  $a$  and  $b$ . One should also keep in mind that the component  $V_a^n = V_{O_a}^n - \beta v^*$  (or  $V_b^n = V_{O_b}^n + \beta v^*$ ) includes both grain displacement and solidification shrinkage.

It is interesting to compute the power dissipation  $\dot{\Omega}$  in the channel by

$$\dot{\Omega} = \{\mathbf{V}\}_b \cdot \{\mathbf{F}\}_b + \{\mathbf{V}\}_a \cdot \{\mathbf{F}\}_a + P_i \Phi_i + P_j \Phi_j \quad (31)$$

or equivalently by

$$\dot{\Omega} = \{\mathbf{U}\}^T [\mathbf{E}] \{\mathbf{U}\} \quad (32)$$

Expanding Eq. (32) using Eq. (29), we obtain

$$\dot{\Omega} = \frac{2h^3}{3\mu L_c} (P_i - P_j)^2 + \mu \left( \frac{L_c}{2h} \right)^3 (V_b^n - V_a^n)^2 + \mu \frac{L_c}{2h} (V_b^t - V_a^t)^2 \quad (33)$$

Thus, the element matrix of the system is positive definite and represents a quadratic form related to dissipation in the channel.

It is convenient to decompose the matrix  $[\mathbf{E}]$  into its symmetric and antisymmetric parts,  $[\mathbf{S}]$  and  $[\mathbf{A}]$ , respectively:

$$[\mathbf{S}] = \begin{pmatrix} +C_1 & -C_1 & 0 & 0 & 0 & 0 \\ -C_1 & +C_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +C_2 & -C_2 & 0 & 0 \\ 0 & 0 & -C_2 & +C_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & +C_3 & -C_3 \\ 0 & 0 & 0 & 0 & -C_3 & +C_3 \end{pmatrix} \quad (34)$$

and

$$[\mathbf{A}] = \begin{pmatrix} 0 & 0 & -L_{ia} & +L_{ib} & +h & +h \\ 0 & 0 & -L_{ja} & +L_{jb} & -h & -h \\ +L_{ia} & +L_{ja} & 0 & 0 & 0 & 0 \\ -L_{ib} & -L_{jb} & 0 & 0 & 0 & 0 \\ -h & +h & 0 & 0 & 0 & 0 \\ -h & +h & 0 & 0 & 0 & 0 \end{pmatrix} \quad (35)$$

Inserting this decomposition into the power dissipation yields

$$\dot{\Omega} = \{\mathbf{U}\}^T ([\mathbf{S}] + [\mathbf{A}]) \{\mathbf{U}\} = \{\mathbf{U}\}^T [\mathbf{S}] \{\mathbf{U}\} \quad (36)$$

since  $\{\mathbf{U}\}^T [\mathbf{A}] \{\mathbf{U}\} \equiv 0$ . The antisymmetric part of  $[\mathbf{E}]$ ,  $[\mathbf{A}]$ , represents coupling between the pressure in the fluid channels and the displacement of the grains. This term does not dissipate energy in our formulation.

This form of the matrix is consistent with the Onsager–Casimir theory of transport phenomena [33]. Consider the two sets of conjugate quantities. One set is invariant under time reversal ( $P_i, P_j, \{\mathbf{F}\}_a, \{\mathbf{F}\}_b$ ), whereas the other set ( $\Phi_i, \Phi_j, \{\mathbf{V}\}_a, \{\mathbf{V}\}_b$ ) changes sign. The symmetric matrix  $[\mathbf{S}]$  couples quantities that have different behavior with respect to time reversal, whereas the anti-symmetric matrix  $[\mathbf{A}]$  couples the quantities with the same behavior. For example,  $\Phi_i$  is related to  $P_i, P_j$  by  $[\mathbf{S}]$  and is related to  $\{\mathbf{V}\}_a, \{\mathbf{V}\}_b$  by  $[\mathbf{A}]$ . It is interesting to note that this fundamental relation is obtained by a simple integration of the fluid flow equations [34]. The usual volume-averaged formulation with the same set of unknowns for describing semi-solid materials (pressure in the liquid, velocity or deformation rate in the solid) does not reveal the symmetries inherent in the present model.

### 3.5. Global problem

To assemble the global problem from the contributions of the individual elements, both the unknown velocities at the grain centers and the resulting forces are expressed in a global coordinate system ( $X, Y$ ) (see Fig. 3). One has, for example:

$$\begin{pmatrix} F_a^X \\ F_a^Y \end{pmatrix} = \begin{pmatrix} n_X & -n_Y \\ n_Y & n_X \end{pmatrix} \begin{pmatrix} F_a^n \\ F_a^t \end{pmatrix} \quad (37)$$

where  $N_X$  and  $N_Y$  are the components of the channel normal vector in the global frame. The pressures and fluxes for each channel in the global coordinate system are obtained by the usual transformation rules *i.e.*,

$$\{\mathbf{W}\}' = [\mathbf{Q}]\{\mathbf{W}\} = [\mathbf{Q}][\mathbf{E}]\{\mathbf{U}\} = [\mathbf{Q}][\mathbf{E}][\mathbf{Q}]^T \{\mathbf{U}\}' = [\mathbf{E}'] \{\mathbf{U}\}' \quad (38)$$

where  $(\{\mathbf{W}\})^T = (\Phi_i, \Phi_j, F_a^X, F_b^X, F_a^Y, F_b^Y)$ ,  $(\{\mathbf{U}\})^T = (P_i, P_j,$

$V_a^X, V_b^X, V_a^Y, V_b^Y)$  and  $[\mathbf{E}]' = [\mathbf{Q}][\mathbf{E}][\mathbf{Q}]^T$ . The transformation matrix  $[\mathbf{Q}]$  is given by:

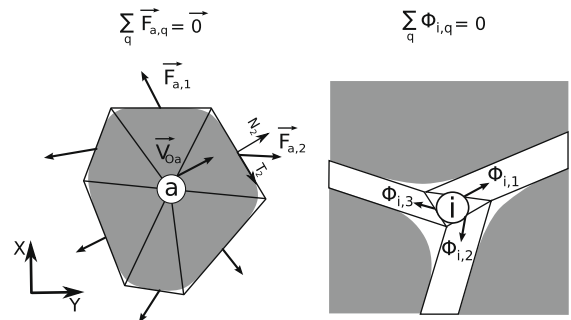


Fig. 3. Construction of the global problem from the elementary matrices. The sum of forces on each grain is zero and the sum of fluxes flowing in and out of each vertex is zero.

$$[\mathbf{Q}] = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & n_X & 0 & -n_Y & 0 \\ 0 & 0 & 0 & n_X & 0 & -n_Y \\ 0 & 0 & n_Y & 0 & n_X & 0 \\ 0 & 0 & 0 & n_Y & 0 & n_X \end{pmatrix} \quad (39)$$

Since  $V_a^n = V_{O_a}^n - \beta v^*$  and  $V_b^n = V_{O_b}^n + \beta v^*$ , Eq. (29) in the  $(X, Y)$  frame becomes

$$\begin{pmatrix} \Phi_i \\ \Phi_j \\ F_a^X \\ F_b^X \\ F_a^Y \\ F_b^Y \end{pmatrix} = [\mathbf{Q}][\mathbf{E}][\mathbf{Q}]^T \begin{pmatrix} P_i \\ P_j \\ V_{O_a}^X \\ V_{O_b}^X \\ V_{O_a}^Y \\ V_{O_b}^Y \end{pmatrix} + [\mathbf{Q}][\mathbf{E}] \begin{pmatrix} 0 \\ 0 \\ -\beta v^* \\ +\beta v^* \\ 0 \\ 0 \end{pmatrix} \quad (40)$$

The last term, which we call  $\{\mathbf{B}\}'$ , is associated with solidification shrinkage and is known from the external solidification model. The balance of mass and force is obtained by summing Eq. (40) over all elements. This procedure is similar to the matrix assembly in the standard finite element method *i.e.*, each contribution associated with a given liquid channel with a local numbering (a, b, i, j) (Section 3.4) is added to the global matricial problem with a global numbering of all the grains and vertices. The result is written in the compact form

$$[\mathbf{E}_{\text{tot}}]'\{\mathbf{U}_{\text{tot}}\}' = -\{\mathbf{B}_{\text{tot}}\}' \quad (41)$$

where the vector of unknowns  $\{\mathbf{U}_{\text{tot}}\}$  contains the velocities of the  $N_g$  grains ( $V_{O_a}^X, V_{O_a}^Y$ ) in the global frame and the pressures  $P_i$  at the  $N_v$  vertices.

Integration points located at the external boundary of the global domain are subject to boundary conditions. An imposed flux on a channel vertex and an imposed force on a grain are Neumann-type boundary conditions in this formulation. These are taken into account by adding the imposed constraint into the global vector  $-\{\mathbf{B}_{\text{tot}}\}'$ . Boundary conditions specifying either the velocity of a grain or an imposed pressure at a channel vertex are essential boundary conditions. These are included in the formulation using a penalty method, as in a standard finite element method.

Finally, the linear system of Eq. (41) is solved with a standard LU decomposition. The velocities computed in the  $\{\mathbf{U}_{\text{tot}}\}$  are used to update the grains positions at the next time step.

### 3.6. Detection of contact

The present model is intended to be used for the study of hot cracking *i.e.*, for  $g_s \gtrsim 0.9$ , so that the width of the liquid channels is very small compared to the grain size and the displacement of the grains is very limited. It is important in the implementation of the model to detect and account for contact between grains. Eq. (9) shows that the pressure drop in a channel tends to infinity as  $(1/h)^3$  as  $h \rightarrow 0$ , and

this is sufficient to prevent the interpenetration of the grains in the simulation as long as the time step is sufficiently small. In some highly constrained situations we found it necessary to implement a dynamic time step refinement procedure in order to prevent grain interpenetration.

It is more problematic to handle the changes of the environment of the grains *i.e.*, modifications of their nearest neighbors. This typically occurs after large displacements of the grains, especially for channels that are short to begin with. There are a few additional situations where the grains can interpenetrate (see Ref. [8] for further details). These cases are handled by revising the list of the first neighbors after each time step [20]. In the example problems presented in the next section, the volume fraction of solid is high and the system is thus sufficiently constrained that this phenomenon does not occur.

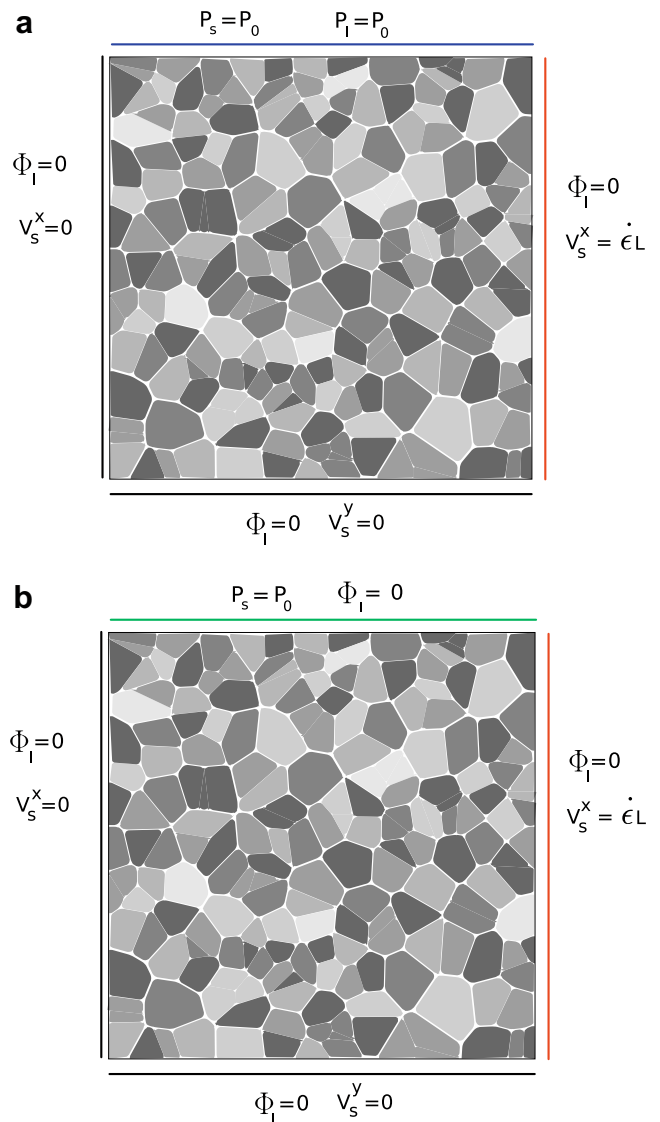


Fig. 4. Boundary conditions for two traction tests along the  $X$  axis: (a) ideal feeding from the upper boundary; (b) no feeding. The grains or clusters of grains are colored with various grey levels.

## 4. Results

### 4.1. Boundary conditions

To use the model to investigate the mechanical behavior of the mushy zone, two test cases were analyzed where a tensile load was applied to a small ensemble of grains comprising a square volume element of edge  $L_V$ . Boundary conditions for the two cases are shown in Fig. 4. Since two phases are present, boundary conditions are needed for either the pressure or the flow rate for the liquid channels, and for either the velocity or the applied forces on the solid grains.

The two cases differ only in the boundary conditions applied on the top surface. In the first case (Fig. 4(a)), a pressure  $P_0$  is imposed on both the liquid and the solid, corresponding to an average hydrostatic pressure on the system.<sup>2</sup> The fluid flow is free, thus allowing feeding from the upper boundary. We refer to this case as “ideal feeding” because it simulates a sample in contact with a liquid reservoir (a feeder) at pressure  $P_0$ . In the second case, we also impose a pressure  $P_0$  on the upper surface of the solid grains but the fluid flow is set to zero. This simulates a situation where feeding is impossible.

The remaining boundary conditions are the same for both cases. The fluid flow and the horizontal  $X$ -component of the grain velocity are zero on the left boundary, while the  $Y$ -component of the grain velocity is free *i.e.*, no forces along the vertical axis. This set of boundary conditions is equivalent to a symmetry plane. On the bottom boundary, the flux and the  $Y$ -component of the velocity are zero while the  $X$ -component is free. On the right boundary, a velocity  $\dot{\epsilon}L_V$  is imposed on the solid in the  $X$ -direction to study the effect of an imposed strain rate  $\dot{\epsilon}$ . The fluid flow is zero on the right boundary.<sup>3</sup>

We note that these boundary conditions are similar to those of the model derived by Lahaie and Bouchard for a regular arrangement of hexagonal grains [35]. In our numerical calculations, the solidification of the system is calculated first, before the mechanics of the mushy zone is computed, without allowing any further solidification *i.e.*, at fixed solid fraction. This implies that  $g_s$  is fixed, so that there is no solidification shrinkage.

### 4.2. Tension tests

Fig. 5(a) shows the stress–strain curves for a sample solidified at constant  $\dot{T} = -1 \text{ K s}^{-1}$ , up to three volume fractions of solid ( $g_s = 0.92, 0.94$  and  $0.96$ ). Each sample was then strained along the  $X$ -direction at a rate

<sup>2</sup> To represent the hydrostatic pressure on the solid, a force is imposed on each grain at the boundary. This force is oriented along the normal to the boundary and is equal to  $-P_0L_b$  where  $L_b$  is the length of the external boundary of the grain.

<sup>3</sup> Note that, for boundary conditions, the liquid flux is considered in the frame of the solid grains. In the laboratory frame, a fluid flux is observed due to the advection of the solid.

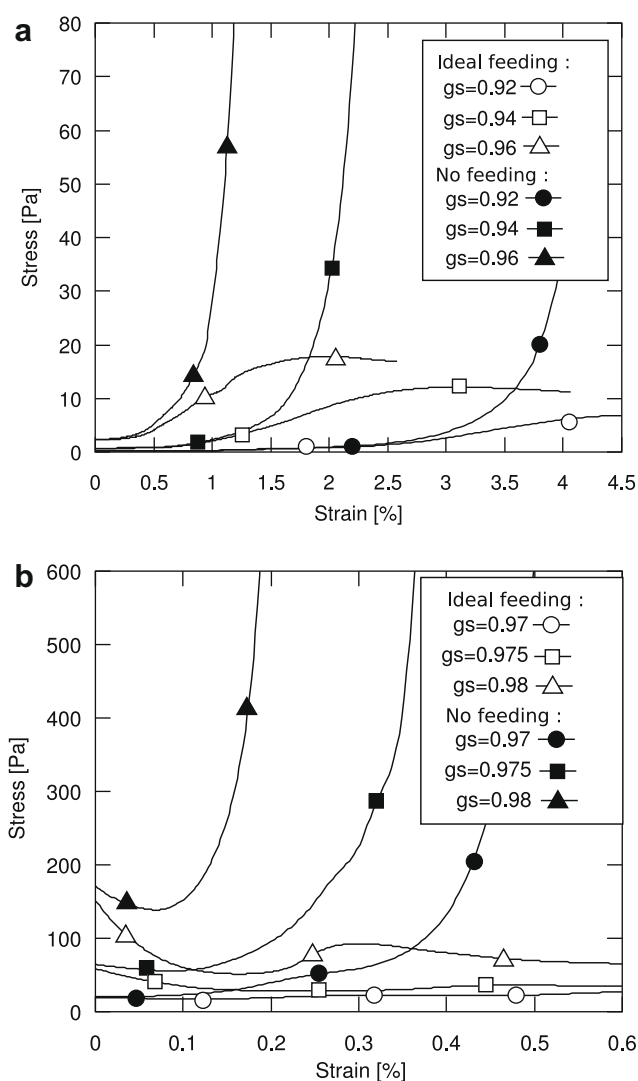


Fig. 5. Stress as a function of strain for a square domain strained at a rate  $\dot{\epsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . Open and filled symbols correspond to ideal and no feeding, respectively. (a)  $g_s < 0.97$ , (b)  $g_s > 0.97$ .

$\dot{\epsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . The results for the two tests, ideal and no feeding, are shown with open and filled symbols, respectively. As can be seen, the two tests give the same stress–strain response at strains up to about 2.5% for  $g_s = 0.92$ , 1.2% for  $g_s = 0.94$  and 0.3% for  $g_s = 0.96$ . Beyond these strains, the stress increases abruptly when feeding is not allowed, whereas it remains low and even decreases past a maximum in the case of ideal feeding.

These results can be understood by looking at the local deformation mechanisms shown in Fig. 6, corresponding to the isothermal mushy zone strained at  $g_s = 0.92$ . This domain contains 200 grains having an average diameter of  $100 \mu\text{m}$ . Note that the computation of a traction test simulation on such a mushy zone takes about 30 s on a personal computer with a 2 GHz Intel Core Duo processor. Fig. 6(1) shows the grain structure with the liquid channels at the onset of deformation *i.e.*, for  $\epsilon = 0$ . The grains are identified by assigning various gray levels, and the velocity of each grain is displayed with small arrows in Fig. 6(1a)



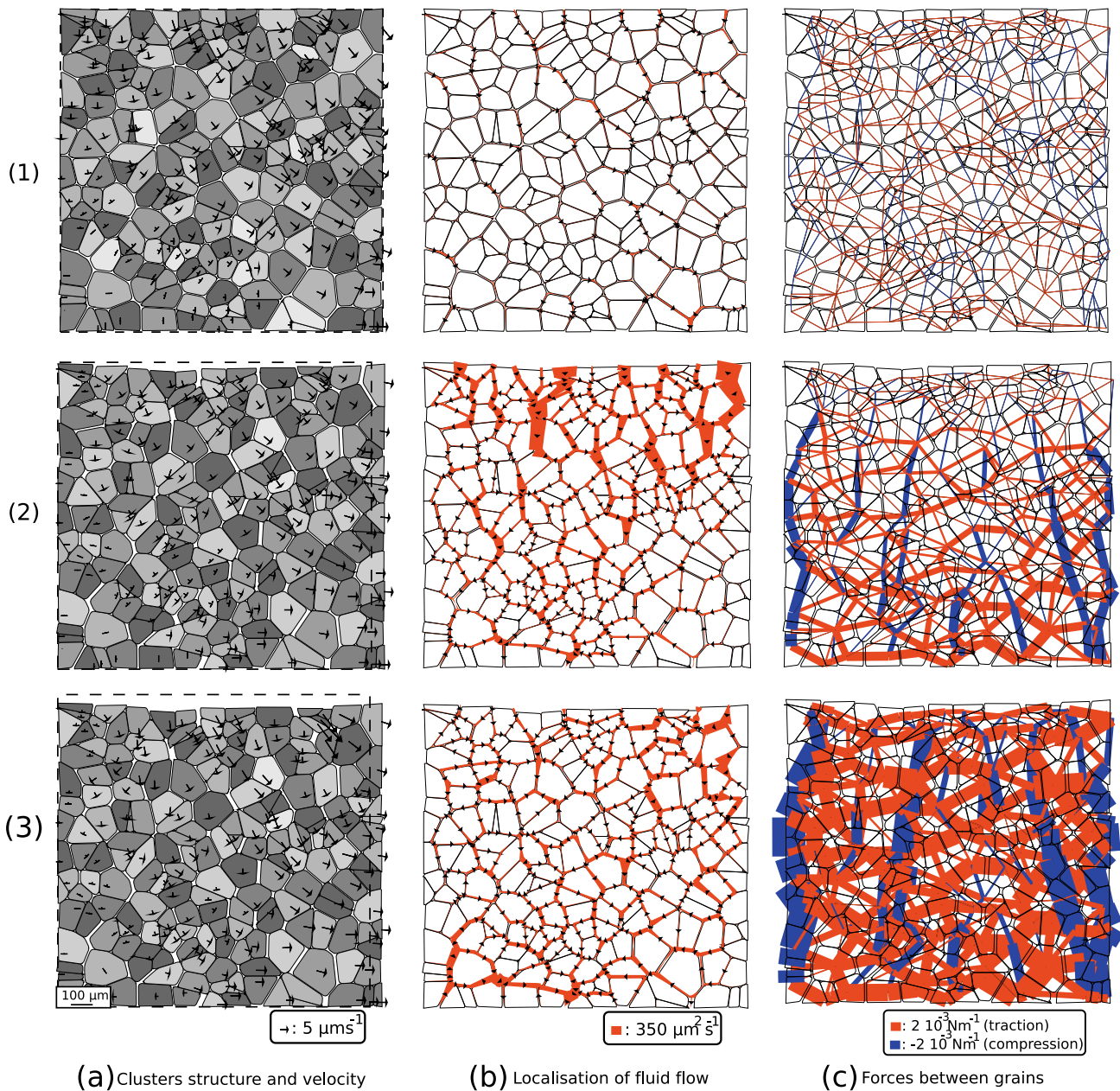


Fig. 6. Isothermal mushy zone with  $g_s = 0.92$  and deformed at a strain rate  $\dot{\epsilon} = 4 \times 10^{-3} s^{-1}$  along the horizontal  $X$ -direction: (1) mushy zone at 0% strain; (2) mushy zone at 4% strain with ideal feeding from the upper face; (3) mushy zone at 4% strain without feeding from the upper face. In (a), the grains (or grain clusters) are shown with various grey levels together with their velocity represented with small arrows. In (b), the flow in the channels is represented with a line of thickness proportional to the intensity and a triangle indicating the direction. In (c), the forces between the grains are represented with lines of variable thickness proportional to the modulus. A grey hue (red) corresponds to traction and a dark hue (blue) to compression. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

(the scale at the bottom of the figure gives the modulus of the velocity). When two grains establish a solid bond *i.e.*, the width of the corresponding channel goes to zero, they are shaded with the same gray scale, making it easy to recognize the formation of grain clusters as solidification progresses [25]. At this relatively low volume fraction of solid ( $g_s = 0.92$ ), only a few such clusters of grains have formed.

In Fig. 6(b), the fluid flow in each channel is represented by lines whose width is proportional to their magnitude, the direction being indicated by a black triangle. The

scale used for this flow representation is again shown at the bottom of the figure. As two grains get closer together, they squeeze the liquid out of the channel; conversely, as they move away from each other, liquid is pumped into the channel. In both cases, the width of the corresponding line varies along the channel length. The flow can also be important in channels of fixed width that feed other regions of the mushy zone. As can be seen in Fig. 6(b), deformation of the mush is accommodated by fluid flow, but these flows remain small and localized. Long-range feeding of

the mush is not necessary at low strain, and therefore both cases give the same behavior of the mush (see Fig. 5).

The stresses in the sample are also very low at low strain, as indicated in Fig. 6(1c). The interaction forces between the grains via the liquid channel are represented by a line connecting nucleation centers, whose width is proportional to the magnitude of the force (scale shown at the bottom), and whose gray scale level (or colour) indicates whether the force is tensile or compressive. At low volume fraction of solid and strain, the forces are very low and the corresponding lines are barely visible in Fig. 6(1c).

Fig. 6(2) shows the same mushy zone after 4% deformation for the ideal feeding case, while Fig. 6(3) shows the case where feeding is prohibited. The overall deformation is indicated in (a), where the initial volume element is drawn as a dashed-line square. It is important to note that deformation is localized to a few channels, roughly oriented normally to the tensile direction. The fluid tends to flow from channels oriented in the direction of the stress to channels oriented perpendicular to the stress. The grains tend to be pulled inward along the vertical  $Y$ -direction as we try to pull the mushy zone in the  $X$ -direction. This is also reflected by the forces shown in Fig. 6(2c) and (3c), which essentially correspond to traction along the horizontal  $X$ -direction and to compression along the  $Y$ -direction.

It is also interesting to note that fluid flow is much more important in the case of ideal feeding (Fig. 6(2b)) compared to the case of no feeding (Fig. 6(3b)), even though the imposed strain rate is the same. This shows that redistribution of fluid occurs over larger distances with the accumulation of deformation. Fluid flow from the upper boundary is clearly visible in Fig. 6(2b), and this flow relaxes the stresses in the upper part of the sample (Fig. 6(2c)).

If the mush cannot be fed from the upper boundary (Fig. 6(3)), redistribution of the fluid channels and of the grains also occurs as deformation increases. However, since no feeding from the top surface is allowed, the fluid follows a more difficult path, and the stresses in the samples are higher. Note that, as no liquid flow is allowed on any boundary for this case and the solid grains are rigid, the total volume of the specimen (grains + liquid) is constant.

In summary, at low strain, deformation is accommodated by local redistribution of the liquid. This deformation is localized in liquid channels oriented roughly perpendicular to the stress direction. As deformation increases, more channels get closed and fluid redistribution occurs on a larger scale. At that point, the ability to feed the mush from some liquid reservoir becomes important.

#### 4.3. Transition in the feeding mechanism

As the volume fraction of solid in the volume element increases, the difference between the ideal-feeding and no-feeding cases occurs at lower strain (Fig. 5). The reason for this is fairly obvious, as the width of the liquid channels decreases with increasing  $g_s$ .

However, for  $g_s > 0.97$  (Fig. 5(b)), the behavior of the two cases is different even at the limit  $\varepsilon \rightarrow 0$ . To understand this new response, consider Fig. 7, which shows a mushy zone with  $g_s = 0.975$  deformed at the same strain rate  $\dot{\varepsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . At the onset of deformation ( $\varepsilon = 0$ , Fig. 7(1a)), it can be seen that the solid grains start to form significant numbers of grain clusters. Moreover, Fig. 7(1b) shows that there is a significant redistribution of fluid, even though the deformation of the mush is zero at that stage. The fluid is located predominantly at the boundaries of the clusters which move as a single larger grain. It is interesting to compare this figure with Fig. 6(1b), which represents a mushy zone under the same straining and feeding conditions but at a lower solid fraction.

The same mushy zone is represented in Fig. 7(2) at 0.05% deformation *i.e.*, after 0.125 s. The very small deformation is localized to just a few channels that are located at the edges of the clusters and oriented normal to the tensile axis. Local redistribution of the liquid is difficult and most of the fluid to accommodate deformation is brought from the upper boundary even at this low strain level. Therefore, above  $g_s = 0.97$ , the deformation mechanism due to local fluid redistribution is no longer possible, due to the presence of relatively large clusters and thinner liquid channels. It is interesting to note that the volume fraction of solid at which the mechanical behavior of the mush changes corresponds precisely to the value  $g_{s,1\%ile}$  at which 1% of the liquid channels become isolated and the permeability of the mush deviates from the Kozeny–Carman relationship [25].

The mechanical model we have presented shows that this solid fraction also corresponds to the point where accommodation of deformation by fluid flow becomes extremely difficult. Therefore, this point can be associated with the ductility minimum point observed experimentally [6,13], also called coalescence solid fraction by some authors [7]. We find this point at a value  $g_s = 0.97$ , whereas the experiments performed on inoculated globular microstructures give instead a value of  $g_s = 0.95$  [7]. This difference is probably due to the 2-D nature of our model, which tends to underestimate the size of the last liquid films (segments in a 2-D Voronoi model instead of polyhedral surfaces in three dimensions).

#### 4.4. Discussion

The effect of external loads on the response in the model can be deduced easily from the linearity of the matrix  $[E]$  (Eq. (29)). In particular, an increase in the metallographic pressure  $P_0$  applied on the upper surface of Fig. 4 simply shifts the stress response of the solid network.<sup>4</sup> This response corresponds to the Terzaghi effective stress *i.e.*,

<sup>4</sup> From a numerical point of view, it is clear that zero grain displacement and a uniform pressure is a solution of the problem. Because the system is linear, this implies that any solution can be shifted by a uniform amount of pressure without affecting the displacement of the grains.

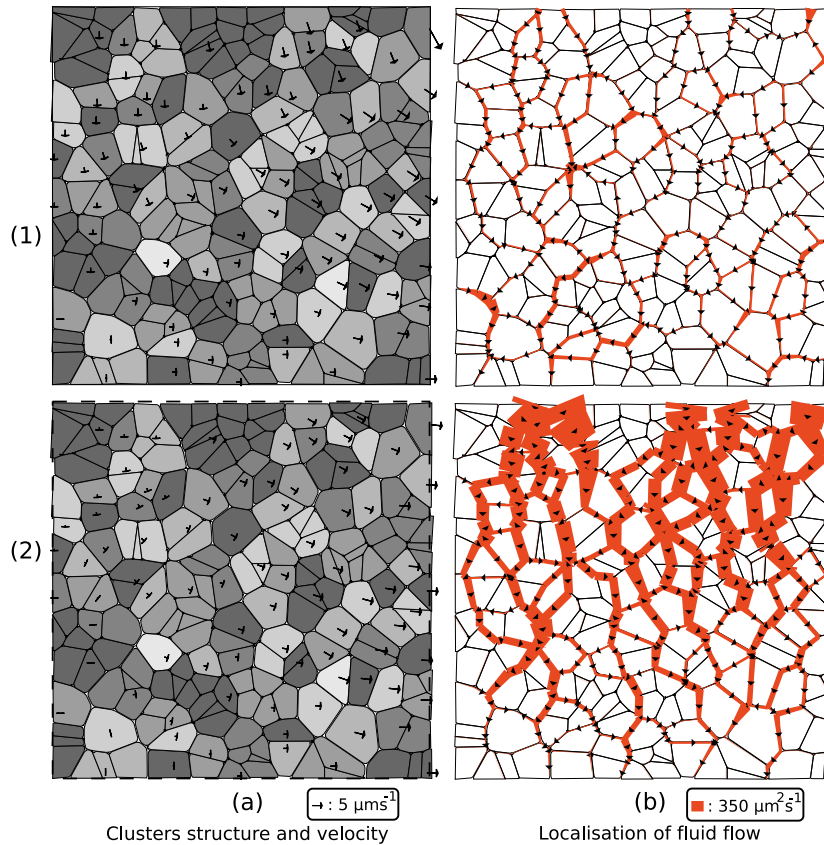


Fig. 7. Isothermal mushy zone with  $g_s = 0.975$  strained with  $\dot{\epsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . Feeding from the upper face is allowed:  $\epsilon = 0$  (1),  $\epsilon = 0.05\%$  (2). In (a), the grains and grain clusters are shown with various grey levels and their velocity is indicated with small arrows. In (b), the flow in the channels is displayed with lines of thickness proportional to the intensity and triangles indicating the direction.

the behavior of the mush depends only on the difference between the applied stress and the hydrostatic pressure [36]. Similarly, the stress response of the mushy zone varies linearly with the strain rate.

On the other hand, the evolution of the mushy zone with strain requires a numerical calculation. The stress–strain curves in Fig. 5 can be compared qualitatively with experimental data (see e.g. [6–8]). For solid fractions lower than  $g_{s,1\%ile}$  (Fig. 5), the strain at which the stress increases abruptly corresponds well to the experimental strains at fracture for the corresponding value of  $g_s$ . However, the shape of the stress–strain curve and the magnitude of the stress are clearly different from the experimental values. At higher solid fractions, the strain at which the stress increases abruptly no longer correlates well with the experimental observations.

We have not considered solid deformation in the model. For a solid fraction lower than the ductility minimum ( $g_s < g_{s,1\%ile}$ ), solid deformation certainly plays a role in the overall behavior of the mush, but grain displacement is the dominant deformation mechanism. The model reproduces the strain at which interlocking of the grains occurs, even though rotations were not considered, but it cannot reproduce the shape of the stress–strain curve. At higher solid fractions ( $g_s > g_{s,1\%ile}$ ), solid deformation is clearly

the dominant mechanism. The ductility increase observed experimentally at high  $g_s$ -value corresponds to the strength increase of the solid network due to its progressive percolation.

This 2-D model demonstrates a transition in the mechanical behaviour of the mush as the solid fraction increases. We have included the 3-D aspects of that transition in a simplified way. Further work is done in our group to extend the present approach to 3-D.

#### 4.5. First consequences on hot tearing criteria

Hot tearing criteria based on the feeding ability of the mush [11,16,12] predict the hot cracking sensitivity of alloys fairly well. Such criteria are based on a critical strain rate, which seems to be particularly applicable in processes such as DC casting, where thermally induced stresses are essentially perpendicular to the thermal gradient [37,38]. However, in tensile test experiments where the applied stress is parallel to the thermal gradient, hot cracking is found to be largely independent of the strain rate [8,38]. As mentioned in the previous section, the response of the present model is at first sight proportional to the strain rate. However, the granular nature of the model makes it strongly strain-dependent.

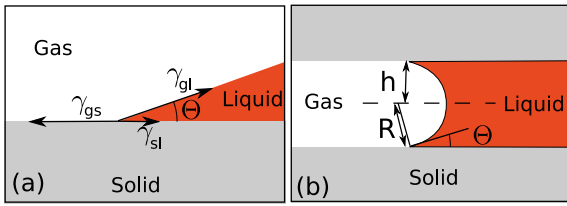


Fig. 8. (a) Equilibrium of forces at triple junction. (b) Shape of the meniscus between two grains.

The criterion for hot tear nucleation is usually written in the form

$$p_l < p_c \quad (42)$$

where  $p_l$  is the local pressure in the liquid and  $p_c$  represents the cavitation pressure at which a pore nucleates. As a first approximation, this cavitation pressure can be estimated as the overpressure required to overcome capillary forces at the liquid–pore interface. Since pores will form at high solid fraction *i.e.*, in very narrow liquid channels, their radius of curvature is dictated by the width of the channel, as illustrated in Fig. 8. At the triple junction between the liquid, solid and pore, the equilibrium condition is given by:

$$\gamma_{gl} \cos \Theta = \gamma_{gs} - \gamma_{sl} \quad (43)$$

where  $\gamma_{sl}$ ,  $\gamma_{gl}$  and  $\gamma_{gs}$  are the interfacial energy between solid and liquid, liquid and pore, and solid and pore, respectively, and  $\Theta$  is the dihedral angle. Therefore, the radius of the pore  $R$  is given by:

$$R = \frac{h}{\cos \Theta} \quad (44)$$

where  $h$  is the half width of the liquid channel (see Fig. 8(b)). Therefore

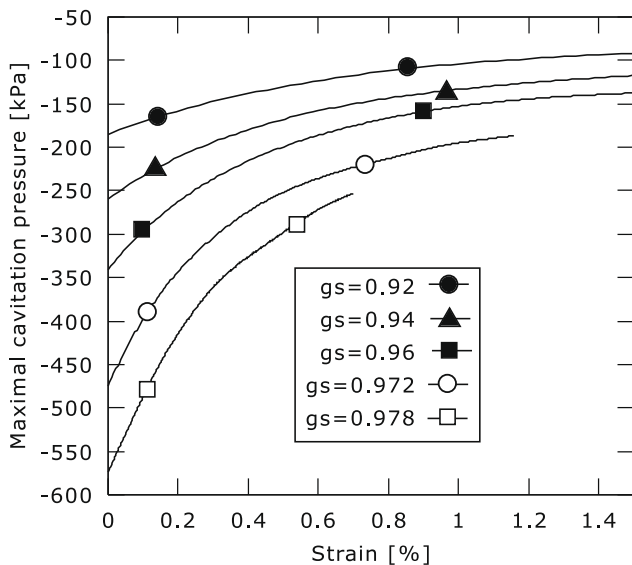


Fig. 9. Maximum value of the cavitation pressure in the mushy zone as a function of strain for an impregnation factor  $I$  of  $1 \text{ J m}^{-2}$ .

$$p_c = \Delta p_\gamma = -\frac{\gamma_{gl}}{R} = -\frac{\cos \Theta \gamma_{gl}}{h} = -\frac{\gamma_{gs} - \gamma_{sl}}{h} = -\frac{I}{h} \quad (45)$$

where  $I$  is called the “impregnation factor”. Since liquid metals wet their own solid very well *i.e.*,  $\gamma_{sl} \ll \gamma_{gl}$ , the value of  $I$  is typically close to  $\gamma_{gl}$  *e.g.*,  $1 \text{ J m}^{-2}$  for Al.

Using such relationships, the maximal cavitation pressure  $p_{c,max}$  is plotted in Fig. 9 as a function of deformation for isothermal mushy zones with various solid fractions deformed at a strain rate  $\dot{\epsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . The pressure corresponds to the pressure necessary for cavitation of a pore in the widest channel of the mush,  $h_{max}$ . This channel width decreases with increasing  $g_s$  and increases considerably with strain, in particular for high solid fraction samples. Note that this evolution is largely independent of the other parameters.

The variations of  $p_c$  due to strain are therefore more important than those induced by the strain rate. This phenomenon can explain the apparent insensitivity of hot cracking to strain rate, at least for tensile test experiments. This idea is further illustrated in Fig. 10, where a mushy zone is represented at various strain levels. In this test, the strain rate  $\dot{\epsilon}$  is equal to  $4 \times 10^{-3} \text{ s}^{-1}$ ,  $g_s = 0.92$  and feeding from the upper boundary is not allowed. The localization of the fluid flow and the grain velocity are represented on the same picture. Channels in which feeding is not represented (white channels) correspond to those in which a pore has nucleated. In order to reach depressions capable of producing a pore by cavitation, the pressure at the upper boundary was fixed to  $P_0 = -120 \text{ kPa}$ . The impregnation factor  $I$  in these simulations was fixed to  $1 \text{ J m}^{-2}$ .

Fig. 10 clearly shows the nucleation of pores in the largest channels, where deformation has been localized. Note that this approach allows an estimation of the appearance of damage in the mushy zone, but cannot model fracture, which would require explicit modeling of the deformation of the solid grains.

## 5. Conclusion

This paper has presented the development of a 2-D granular model for the mechanical behavior of mushy zones that brings valuable insight into the interrelations between intergranular flow and grain movement. The model is based on conservation of mass and force at the level of the intergranular region. It produces naturally a form that is consistent with non-equilibrium thermodynamics. The whole mechanical problem can thus be expressed as a minimization of dissipation. Therefore, the results of the present simulations are well suited for continuum models based on a dissipation potential [7].

The model accounts directly for the random nature of grain nucleation, and for the progressive formation of grain clusters during solidification [25]. In addition, the granular nature of the material is modeled, which leads to further localization of deformation and feeding (besides the localization due to grain clusters). Both of these impor-

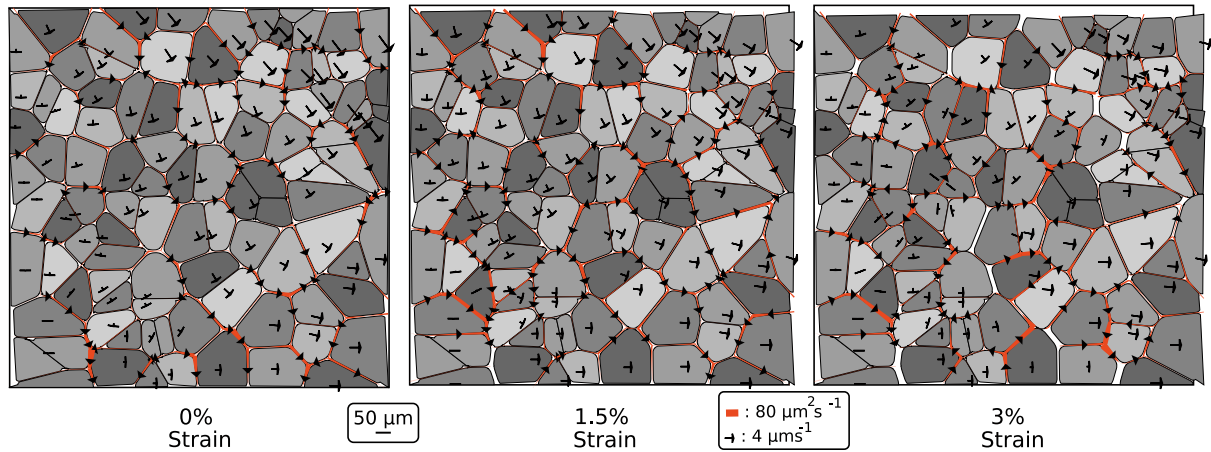


Fig. 10. Mushy zone at various strain levels with  $g_s = 0.92$  and  $\dot{\epsilon} = 4 \times 10^{-3} \text{ s}^{-1}$ . Feeding from the upper face is not allowed. Grain velocity (black arrows) and fluid flow (grey/red lines) are represented on the same picture. The channels on which feeding is not represented (white channels) correspond to those where a pore has nucleated. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

tant phenomena cannot be resolved using typical volume-averaged formulations that smear out the details of the grain structure.

The formulation of the model requires only a few integration points for each grain. Computation times are therefore very low and leave room for further extensions, in particular to three dimensions.

#### Acknowledgement

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#### Appendix A. Scaling analysis and simplification of the equations

The  $X$ -component of the momentum balance for a constant density Newtonian fluid in a 2-D liquid channel is given by

$$\rho_l \left( \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial X} + v_y \frac{\partial v_x}{\partial Y} \right) = \rho_l \frac{Dv_x}{Dt} = - \frac{\partial p}{\partial X} + \mu \left( \frac{\partial^2 v_x}{\partial X^2} + \frac{\partial^2 v_x}{\partial Y^2} \right) \quad (46)$$

We follow the procedures in Ref. [39] to put this equation in dimensionless form. To that end, we define the following scaled variables:

$$X^\circ = \frac{X}{L_c}, \quad Y^\circ = \frac{Y}{2h}, \quad v_x^\circ = \frac{v_x - V_a^t}{V^t}, \quad v_y^\circ = \frac{v_y - V_a^n}{V^n}, \quad (47)$$

$$t^\circ = \frac{tV^t}{L_c}, \quad p^\circ = \frac{p - P_i}{\Delta P_X}$$

where  $V^t = (V_b^t - V_a^t)$ ,  $V^n = (V_b^n - V_a^n)$  and  $\Delta P_X = (P_j - P_i)$ .

Substituting these scaled variables into Eq. (46) gives

$$\frac{4h^2 \rho_l V_T}{\mu L_c} \frac{Dv_x^\circ}{Dt^\circ} = - \frac{4h^2 \Delta P_X}{\mu V_T L_c} \frac{\partial p^\circ}{\partial X^\circ} + \frac{4h^2}{L_c^2} \frac{\partial^2 v_x^\circ}{\partial X^{\circ 2}} + \frac{\partial^2 v_x^\circ}{\partial Y^{\circ 2}} \quad (48)$$

The factor  $2h/L_c$  that appears in several terms can be expressed in terms of the solid fraction  $g_s$ :

$$\frac{2h}{L_c} = 2 \frac{H_{tot}}{L_{tot}} \left( \frac{1 - g_s^{1/2}}{g_s^{1/2}} \right) \quad (49)$$

where  $H_{tot}$  is the height of the elementary triangle and  $L_{tot}$  is the length of its base. For a regular hexagonal network of solid grains this is constant, given by

$$\frac{2h}{L_c} = \sqrt{3} \left( \frac{1 - g_s^{1/2}}{g_s^{1/2}} \right) \quad (50)$$

which is precisely the term introduced by Lahaie and Bouchard in their hot tearing criterion [35]. We are interested in solid fractions  $g_s \gtrsim 0.8$  for which  $(g_s^{-1/2} - 1) \sim (1 - g_s)/2 \lesssim 0.1$ .

To estimate the relative magnitude of the various terms, we consider the typical values of the physical parameters in an inoculated Al–Cu alloy  $\rho_l \sim 2440 \text{ kg m}^{-3}$ ,  $\mu \sim 1.5 \times 10^{-3} \text{ Pa s}$ ,  $L_c \sim 10^{-4} \text{ m}$  [40]. Moreover, in DC casting the typical strain rate is on the order of  $\dot{\epsilon} \sim 10^{-3} \text{ s}^{-1}$  [2] and thus  $V^t \sim L_c \dot{\epsilon} \sim 10^{-7} \text{ m s}^{-1}$ . Thus

$$\frac{4h^2 \rho_l V^t}{\mu L_c} \sim 10^{-6} \ll 1 \quad (51)$$

and the transient and inertial terms of Eq. (48) are negligible. Similarly,

$$\frac{4h^2}{L_c^2} \sim 10^{-2} \ll 1 \quad (52)$$

and we can reasonably neglect the term in  $\partial^2 v_x / \partial X^2$ . This leaves the simplified equation describing the flow in a channel:

$$\frac{\partial^2 v_x^\circ}{\partial Y^{\circ 2}} = \frac{4h^2 \Delta P_X}{\mu V^t L_c} \frac{\partial p^\circ}{\partial X^\circ} \quad (53)$$

Applying the same procedure to the equation for the  $Y$ -component of the fluid velocity gives:

$$\frac{\partial^2 v_Y^\circ}{\partial Y^\circ} = \frac{2h\Delta P_Y}{\mu V^n} \frac{\partial p^\circ}{\partial Y^\circ} \quad (54)$$

To estimate of the pressure variation in the channel, we set the dimensionless groups to one [39]:

$$\Delta P_X \sim \frac{\mu V^t L_c}{4h^2}, \Delta P_Y \sim \frac{\mu V^n}{2h} \quad (55)$$

and thus

$$\frac{\Delta P_Y}{\Delta P_X} \sim \frac{2h}{L_c} \quad (56)$$

Thus, to a first approximation, we can neglect the variation of pressure across the channel in comparison to the variation of pressure along the channel. Therefore, even though fluid flow exists in the  $Y$ -direction due to solidification shrinkage or grain displacement, the Poiseuille equation gives a good approximation of the flow.

In the derivation of the model, we considered only the dissipation along the channels and neglected the dissipation at triple junctions. Indeed, the dissipation along the channels is mainly due to viscous losses, whereas the dissipation at triple junctions is due to the direction change of the flow. Such losses are proportional to the kinetic energy of the flow [41]. However, Eq. (51) shows that the ratio between kinetic energy and viscous dissipation (Reynolds number) is on the order of  $10^{-5}$  and therefore it is reasonable to neglect the dissipation at triple junctions.

## Appendix B. Detailed integration of the constitutive equations

### B.1. Basic equations

Considering that  $\partial p/\partial X$  is constant along the width of the channel (see Appendix A), the integration of Eq. (3) (see main section) gives:

$$v_X(X, Y) = \frac{1}{2\mu} \frac{\partial p}{\partial X} (Y^2 - h^2) + \frac{V'_b - V'_a}{2h} Y + \frac{V'_b + V'_a}{2} \quad (57)$$

where a non-slip condition is considered at the  $s - \ell$  interfaces. Therefore, we have:

$$\Phi_{i \rightarrow j}(X) = -\frac{2}{3\mu} \frac{\partial p}{\partial X} h^3 \quad (58)$$

and from Eq. (6) we get:

$$\frac{2h^3}{3\mu} \frac{\partial^2 p}{\partial X^2} = V^n \quad (59)$$

where the source term  $V^n$  for the flow in the channel is given by:

$$V^n = V_b^n - V_a^n = V_{O_b}^n - V_{O_a}^n + 2\beta v^* \quad (60)$$

Finally, the pressure and velocity profiles are given by:

$$p(X) = \frac{3\mu V^n}{4h^3} \left( X^2 - \left( \frac{L_c}{2} \right)^2 \right) + \frac{P_j - P_i}{L_c} X + \frac{P_i + P_j}{2} \quad (61)$$

$$v_X(X, Y) = \left( \frac{3V^n}{4h^3} X + \frac{P_j - P_i}{2\mu L_c} \right) (Y^2 - h^2) + \frac{V'_b - V'_a}{2h} Y + \frac{V'_b + V'_a}{2} \quad (62)$$

The integration of Eq. (62) gives the fluid flux in the channel:

$$\Phi_{i \rightarrow j}(X) = -V^n X + \frac{2h^3}{3\mu L_c} (P_i - P_j) + 2h \frac{V'_b + V'_a}{2} \quad (63)$$

### B.2. Liquid flux

The mass balance in each channel must be completed by a mass balance at each vertex. As the fluid is considered incompressible, one has

$$\sum_s \Phi_i^s = 0 \quad (64)$$

where the summation is carried out over the three channels  $s = 1, 2, 3$  connected to vertex  $i$  (see Fig. 3). It is possible to show that this summation is equivalent to [8]

$$\sum_s \frac{2(h^s)^3}{3\mu L_c^s} (P_i - P_j) + 2h^s \frac{V'_b + V'_a}{2} + L_{ib} V_b^n - L_{ia} V_a^n = 0 \quad (65)$$

where the indices of the grains ( $a$  and  $b$ ) correspond to the neighbors of each channel.

### B.3. Forces

In order to get a representation of the stress tensor, let us consider the pressure variation in the  $Y$ -direction. For an incompressible fluid, we have

$$\nabla \cdot \{v\} = 0 \quad (66)$$

As the speed profile along the  $X$ -axis is already defined (Eq. (62)), we get

$$\frac{\partial v_Y}{\partial Y} = -\frac{\partial v_X}{\partial X} = -\frac{3V^n}{4h^3} (Y^2 - h^2) \quad (67)$$

Thus

$$v_Y = -\frac{V^n}{4h^3} Y^3 + \frac{3V^n}{4h} Y + \frac{V_b^n + V_a^n}{2} \quad (68)$$

The variation of pressure in the  $Y$ -direction is obtained from the momentum balance equation,

$$\frac{\partial p}{\partial Y} = \mu \frac{\partial^2 v_Y}{\partial Y^2} \quad (69)$$

We get the variation of pressure along the  $Y$ -direction

$$p = -\frac{3V^n}{4h^3} Y^2 + f(X) \quad (70)$$

where  $f(X)$  is the pressure in the channel for the line  $Y = 0$ , which we take to be equal to the pressure profile of Eq. (61). Finally, the pressure profile is:

$$p(X, Y) = \frac{3\mu V^n}{4h^3} \left( X^2 - \left( \frac{L_c}{2} \right)^2 - Y^2 \right) + \frac{P_j - P_i}{L_c} X + \frac{P_i + P_j}{2} \quad (71)$$

As shown in the scaling analysis, the pressure loss in the  $Y$ -direction is negligible in comparison to the pressure variation in the  $X$ -direction. Note that we found here the relationship  $\Delta P_Y / \Delta P_X \sim h^2 / L_c^2$  whereas the scaling analysis gives a relationship  $\Delta P_Y / \Delta P_X \sim h / L_c$  (Eq. (56)).

The stress tensor in the liquid can be derived from

$$[\sigma](X, Y) = \begin{pmatrix} -p + 2\mu \frac{\partial v_x}{\partial X} & \mu \left( \frac{\partial v_x}{\partial Y} + \frac{\partial v_y}{\partial X} \right) \\ \mu \left( \frac{\partial v_x}{\partial Y} + \frac{\partial v_y}{\partial X} \right) & -p + 2\mu \frac{\partial v_y}{\partial Y} \end{pmatrix} \quad (72)$$

and thus

$$[\sigma](X, Y) = \begin{pmatrix} -p + \frac{3\mu V^n}{2h^3} (Y^2 - h^2) & \left( \frac{3\mu V^n}{2h^3} X + \frac{P_j - P_i}{L_c} \right) Y + \mu \frac{V'_b - V'_a}{2h} \\ \mu \left( \frac{\partial v_x}{\partial Y} + \frac{\partial v_y}{\partial X} \right) & -p - \frac{3\mu V^n}{2h^3} (Y^2 - h^2) \end{pmatrix} \quad (73)$$

where  $p$  is given by Eq. (71). Note that the  $\partial_X v_Y$  term is nil. This stress field is coherent, as we can check that:

$$\nabla \cdot [\sigma](X, Y) = \{\mathbf{0}\} \quad (74)$$

For the simplicity of the equations, we choose to neglect the variation of pressure in the  $Y$ -direction (Eq. (61)). Thus, we should also neglect the  $Y^2$  terms in the diagonal of the stress tensor as they are exactly of the same order.

$$[\sigma](X, Y) = \begin{pmatrix} -p & \left( \frac{3\mu V^n}{2h^3} X + \frac{P_j - P_i}{L_c} \right) Y + \mu \frac{V'_b - V'_a}{2h} \\ \mu \left( \frac{\partial v_x}{\partial Y} + \frac{\partial v_y}{\partial X} \right) & -p \end{pmatrix} \quad (75)$$

Note that the divergence of this tensor is not zero. However, considering this stress tensor, the sum of forces and of rotational momentum on the boundaries of a channel are zero, which is the condition for the coherency of the numerical scheme.

Eq. (75) gives the stress tensor in the part of the channel where the two grains match. In the part where they do not match, we simply consider that we have a homogeneous pressure equal to the pressure of the integration point ( $P_i$  or  $P_j$ ; see Fig. 2). Thus, we can integrate the force exerted by a grain on the liquid

$$\{\mathbf{F}_a\} = \begin{pmatrix} (P_j - P_i)h - \mu \frac{L_c}{2h} (V'_b - V'_a) \\ -\mu \left( \frac{L_c}{2h} \right)^3 V^n + P_i L_{ia} + P_j L_{ja} \end{pmatrix} \quad (76)$$

and

$$\{\mathbf{F}_b\} = \begin{pmatrix} (P_j - P_i)h + \mu \frac{L_c}{2h} (V'_b - V'_a) \\ \mu \left( \frac{L_c}{2h} \right)^3 V^n - P_i L_{ib} - P_j L_{jb} \end{pmatrix} \quad (77)$$

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