Developping the interfacial terms in the averaged mass balance for a solidification shrinkage configuration

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1 What is shrinkage ?

Shrinkage, in its simplest definition, is the volume decrease/contraction of a body. In the context of solidification, we speak of *solidification shrinkage*. Three factors may contribute to this phenomenon, often simultaneously:

- $\rho^l \neq \rho^s$: density jump between the solid and liquid phase (even if these are constant). This is type 1 (T1)
- $\rho^l\left(T, \langle w\rangle^l\right)$: liquid density variations with temperature and the intrinsic average composition of the liquid. This is type 2 (T2)
- $\rho^s\left(T, \langle w\rangle^s\right)$: solid density variations with temperature and the intrinsic average composition of the solid. This is type 3 (T3)

2 Modeling shrinkage

Three scenarions are treated in this report. The first scenario considers only T1 shrinkage. The second considers T1 and T2, while the third scenario considers all three types simultaneously. First, let us introduce the mass balance, averaged over each phase with the interfacial transfer terms.

$$\frac{\partial}{\partial t}\left(g^l\rho^l\right) + \nabla\cdot\left(g^l\rho^l\vec{v}^l\right) = S_V\langle\rho^l\vec{v}^{l^*}\cdot\vec{n}\rangle^* - S_V\langle\rho^l\vec{v}^*\cdot\vec{n}\rangle^* \tag{1a}$$

$$\frac{\partial}{\partial t}\left(g^s\rho^s\right) + \nabla\cdot\left(g^s\rho^s\vec{v}^s\right) = -S_V\langle\rho^s\vec{v}^{s^*}\cdot\vec{n}\rangle^* + S_V\langle\rho^s\vec{v}^*\cdot\vec{n}\rangle^* \tag{1b}$$

where $S_V = A_{sl}/V_{RVE}$ is the specific surface area, $\vec{v}^{l^*}$ and $\vec{v}^{s^*}$ are respectively, the liquid and solid phase velocity at the interface and $\vec{v}^*$ is the solid-liquid interface velocity. For instance, the first RHS term is expanded as follows [Dan2009]:

$$S_V\langle\rho^l\vec{v}^{l^*}\cdot\vec{n}\rangle^* = \frac{A_{sl}}{V_{RVE}}\left(\frac{1}{A_{sl}}\int_{A_{sl}}\rho^l\vec{v}^{l^*}\cdot\vec{n}\,dA\right) \tag{2a}$$

$$= \frac{1}{V_{RVE}}\int_{A_{sl}}\rho^l\vec{v}^{l^*}\cdot\vec{n}\,dA \tag{2b}$$

Summing equations (1a) and (1b), results in the overall mass balance in the RVE:

$$\frac{\partial}{\partial t}\left(g^l\rho^l + g^s\rho^s\right) + \nabla\cdot\left(g^l\rho^l\vec{v}^l + g^s\rho^s\vec{v}^s\right) = S_V\left\langle\rho^l\left(\vec{v}^{l^*} - \vec{v}^*\right)\cdot\vec{n}\right\rangle^* - S_V\left\langle\rho^s\left(\vec{v}^{s^*} - \vec{v}^*\right)\cdot\vec{n}\right\rangle^* \tag{3a}$$

$$\frac{\partial}{\partial t}\left(g^l\rho^l + g^s\rho^s\right) + \nabla\cdot\left(g^l\rho^l\vec{v}^l + g^s\rho^s\vec{v}^s\right) = S_V\left\langle\rho^l\left(\vec{v}^{l^*}\right)\cdot\vec{n}\right\rangle^* - S_V\left\langle\rho^s\left(\vec{v}^{s^*}\right)\cdot\vec{n}\right\rangle^* - S_V\left\langle\left(\rho^s + \rho^l\right)\vec{v}^*\cdot\vec{n}\right\rangle^* \tag{3b}$$

2.1 First scenario: T1

2 main assumptions are made:

- the solid phase is fixed ($\vec{v}^s = \vec{0}$)
- the solid and liquid densities are constant but not equal

Under these assumptions, we may rewrite the mass balance for the liquid phase:

$$\rho^l \frac{\partial g^l}{\partial t} + \nabla \cdot \left(g^l \rho^l \vec{v}^l\right) = \rho^l S_V \left\langle \left(\vec{v}^{l^*} - \vec{v}^*\right) \cdot \vec{n} \right\rangle^* \tag{4a}$$

$$\frac{\partial g^l}{\partial t} + \nabla \cdot \left(g^l \vec{v}^l\right) = S_V \left\langle \left(\vec{v}^{l^*} - \vec{v}^*\right) \cdot \vec{n} \right\rangle^* \tag{4b}$$

$$\nabla \cdot \left(g^l \vec{v}^l\right) = \frac{\partial g^s}{\partial t} + S_V \left\langle \left(\vec{v}^{l^*} - \vec{v}^*\right) \cdot \vec{n} \right\rangle^* \tag{4c}$$

Repeating the same procedure for the solid gives: Under these assumptions, we may rewrite the mass balance for the liquid phase:

$$\rho^s \frac{\partial g^s}{\partial t} + \cancel{\nabla \cdot \left(g^s \rho^s \vec{v}^s\right)} = \cancel{-S_V \left\langle \rho^s \vec{v}^{s^*} \cdot \vec{n} \right\rangle^*} + S_V \left\langle \rho^s \vec{v}^* \cdot \vec{n} \right\rangle^* \tag{5a}$$

$$\frac{\partial g^s}{\partial t} = S_V \left\langle \vec{v}^* \cdot \vec{n} \right\rangle^* \tag{5b}$$

Inserting equation (5b) in (4c) yields:

$$\nabla \cdot \left(g^l \vec{v}^l\right) = S_V \left\langle \vec{v}^* \cdot \vec{n} \right\rangle^* + S_V \left\langle \left(\vec{v}^{l^*} - \vec{v}^*\right) \cdot \vec{n} \right\rangle^* \tag{6a}$$

$$\boxed{\nabla \cdot \left(g^l \vec{v}^l\right) = \nabla \cdot \left\langle \vec{v}^l \right\rangle = S_V \left\langle \vec{v}^{l^*} \cdot \vec{n} \right\rangle^*} \tag{6b}$$

$$\tag{6c}$$

We have averaged the mass balance separately in each phase to find equation (6b). Now, we will start from the mass balance averaged over the RVE containing both phases:

$$\frac{\partial \langle \rho \rangle}{\partial t} + \nabla \cdot \langle \rho \vec{v} \rangle = 0 \tag{7a}$$

$$\frac{\partial}{\partial t}\left(g^l \rho^l + g^s \rho^s\right) + \nabla \cdot \left(g^l \rho^l \vec{v}^l\right) = 0 \tag{7b}$$

$$g^l \cancel{\frac{\partial \rho^l}{\partial t}} + \rho^l \frac{\partial g^l}{\partial t} + g^s \cancel{\frac{\partial \rho^s}{\partial t}} + \rho^s \frac{\partial g^s}{\partial t} + \rho^l \nabla \cdot \left(g^l \vec{v}^l\right) + g^l \vec{v}^l \cdot \cancel{\vec{\nabla} \rho^l} = 0 \tag{7c}$$

$$\left(\rho^l - \rho^s\right) \frac{\partial g^l}{\partial t} + \rho^l \nabla \cdot \left(g^l \vec{v}^l\right) = 0 \tag{7d}$$

$$\boxed{\nabla \cdot \left(g^l \vec{v}^l\right) = \nabla \cdot \left\langle \vec{v}^l \right\rangle = \frac{\rho^l - \rho^s}{\rho^l} \frac{\partial g^s}{\partial t}} \tag{7e}$$