Formulation of Conservation Equations for the Shrinkage-Induced Surface Deformation

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Todo list

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1 Abstract

This report summarizes the derivation of conservation equations (mass, momentum, energy and species) relative to a specific solidification scenario where the surface of the solidifying alloy in contact with a surrounding gas (ambient air, argon gas ...) deforms due to solidification shrinkage, that is, the effect of relative change in density between the liquid and the solid phases of the metal. The shrinkage phenomenon is manifested in 2 important locations, as depicted in figure 1b. First, at the level of the liquid-solid interface in the mushy zone, the solid forms with a density smaller than the liquid's. The volume difference tends to create voids with a big negative pressure, that systematically drains the liquid in its direction. Afterwards, we can see the consequence far away, at the surface ingot, where the initial metal(liquid)-air deforms gradually, forming the so-called *shrinkage pipe*. Since the mass of the alloy and its chemical species are conserved, a density difference between the phases ($\rho^s > \rho^l$), leads to a different overall volume ($V^s < V^l$), once solidification is complete, as shown in the following equations:

$$\rho^l V^l = \rho^s V^s \tag{1a}$$

$$V^s = \frac{\rho^l}{\rho^s} V^l \tag{1b}$$

2 Mass Conservation

2.1 Assumptions

- Two phases are considered, liquid l and solid s: $g^l + g^s = 1 \implies \frac{dg^l}{dt} = -\frac{dg^s}{dt}$

- The phase densities are constant but not equal: $\rho^l = cst_1$ and $\rho^s = cst_2$. Thermal and solutal expansion/contraction is neglected

- The solid phase is assumed static: $\vec{v^s} = \vec{0}$, which yields the following consequences:

    1. $\langle \vec{v} \rangle = g^l \vec{v^l} + g^s \vec{v^s}^{\,0} = g^l \vec{v^l}$
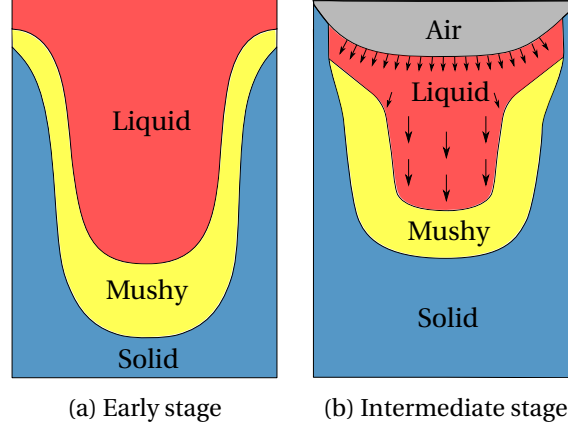
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Figure 1: Schematic of a two cooling stages of an ingot against side and bottom mould walls (not shown). The top surface is free

2. $\langle \rho \vec{v} \rangle = g^l \rho^l \vec{v}^l + \cancel{g^s \rho^l \vec{v}^s}^{\,0} = g^l \rho^l \vec{v}^l$

3. $\frac{\partial \rho^l}{\partial t} = \frac{\partial \rho^s}{\partial t} = 0$

4. $\vec{\nabla} \rho^l = \vec{\nabla} \rho^s = \vec{0}$

2.2 Formulation

The mass balance equation averaged over the two phases, is developed taking into account the assumptions made earlier.

$$\frac{\partial \langle \rho \rangle}{\partial t} + \nabla \cdot \langle \rho \vec{v} \rangle = 0 \tag{2a}$$

$$\frac{\partial}{\partial t}\left(g^l \rho^l + g^s \rho^s\right) + \nabla \cdot \left(g^l \rho^l \vec{v}^l\right) = 0 \tag{2b}$$

$$g^l \cancel{\frac{\partial \rho^l}{\partial t}} + \rho^l \frac{\partial g^l}{\partial t} + g^s \cancel{\frac{\partial \rho^s}{\partial t}} + \rho^s \frac{\partial g^s}{\partial t} + \rho^l \nabla \cdot \left(g^l \vec{v}^l\right) + g^l \vec{v}^l \cdot \cancel{\vec{\nabla} \rho^l} = 0 \tag{2c}$$

$$\left(\rho^l - \rho^s\right) \frac{\partial g^l}{\partial t} + \rho^l \nabla \cdot \left(g^l \vec{v}^l\right) = 0 \tag{2d}$$

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

2.3 Discussion

With the assumptions of static solid phase and constant unequal phase densities, the average mass balance states that the divergence of the liquid velocity is proportional to the solidification rate, the proportionality constant being the relative density change (which results in a relative volume change). This relation between the liquid velocity and the temporal derivative of the solid fraction, explains the flow due to shrinkage. In metallic alloys, the solid density is usually greater than the liquid density, therefore the first term in the RHS is negative. As for the second term, if we neglect remelting, then it'll be positive in the solidifying areas of the alloy. A negative divergence term in these areas, means that a liquid feeding is necessary to compensate for the density difference, hence acting as a flow driving force in the melt. In the case of constant densities, we can easily deduce that the divergence term is null, and therefore no flow is induced by solidification.

Numerically speaking, a non-zero divergence term in the mass balance is equivalent to a compressible fluid behaviour. Additional terms should appear in the other conservation equations, balancing the volume change in the momentum, heat and species transport.

3 Momentum Conservation

In a typical volume averaging approach, one would write one momentum conservation equation for each phase. Nonetheless, only one equation will be present in our case, and that is the consequence of the assumption of the static solid, made in the previous section. It should be emphasized that, despite considering a single conservation equation, the effect of the solid movement with respect to the liquid's can still be incorporated through the interfacial fluxes in the momentum conservation of the liquid phase.

3.1 Assumptions

- The interfacial momentum transfer between the solid and liquid phases is modelled by a momentum flux vector $\vec{\Gamma}^l$, consisting of hydrostatic and deviatoric parts, such that:

$$\vec{\Gamma}^l = \vec{\Gamma}^l_p + \vec{\Gamma}^l_{\mathbb{S}} \tag{4a}$$

$$\vec{\Gamma}^l_p = p^{l^*}\vec{\nabla}g^l = p^l\vec{\nabla}g^l \tag{4b}$$

$$\vec{\Gamma}^l_{\mathbb{S}} = -g^{l^2}\mu^l\mathbb{K}^{-1}\left(\vec{v}^l - \vec{v}^{\mathscr{s}}\right) \tag{4c}$$

where p^{l^*} is the pressure at the interface, considered to be equal to the liquid hydrostatic pressure, $\mathbb{K}$ is the permeability computed by the Carman-Kozeny relation and μ^l is the liquid's dynamic viscosity. For the solid phase, the interfacial terms are the opposite, which cancels them out with the liquid terms if the phase momentum equations are summed up.

- The liquid is considered as a *compressible* Newtonian fluid. It implies that the deviatoric part, $\underline{\mathbb{S}}^l$, of the Cauchy stress tensor is decomposed as follows:

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$$\langle\underline{\sigma}^l\rangle = -\langle p^l\rangle\underline{\mathbb{I}} + \langle\underline{\mathbb{S}}^l\rangle \tag{5a}$$

$$\langle\underline{\sigma}^l\rangle = -\langle p^l\rangle\underline{\mathbb{I}} + 2\mu^l\langle\underline{\dot{\varepsilon}}^l\rangle + \langle\underline{\tau}^l\rangle \tag{5b}$$

where $\langle\underline{\dot{\varepsilon}}^l\rangle$ is the strain rate tensor that depends on the average liquid velocity:

$$\langle\underline{\dot{\varepsilon}}^l\rangle = \underline{\nabla}\langle\vec{v}^l\rangle + \underline{\nabla}^{\mathbf{t}}\langle\vec{v}^l\rangle \tag{6}$$

and $\underline{\tau}^l$ is the extra stress tensor in the liquid, given by:

$$\langle\underline{\tau}^l\rangle = -\lambda\nabla\cdot\langle\vec{v}^l\rangle\underline{\mathbb{I}} \tag{7a}$$

where λ is a dilatational viscosity [Rap2003]. For an incompressible flow, the divergence term vanishes, hence the classical Newtonian constitutive law is retrieved. In the literature, the coefficient λ is taken proportional to the viscosity: $\lambda = \frac{2}{3}\mu^l$

3.2 Formulation

The momentum conservation equation in the liquid writes:

$$\frac{\partial}{\partial t}\left(\rho^l g^l \vec{v}^l\right) + \vec{\nabla}\cdot\left(\rho^l g^l \vec{v}^l \times \vec{v}^l\right) = \vec{\nabla}\cdot\left(g^l \underline{\sigma}^l\right) + g^l \vec{F}_{\mathrm{v}} + \vec{\Gamma}^l \tag{8}$$

where $\vec{F}_{\mathrm{v}}$ is an external volume force. The effect of the mass balance obtained in the previous section is incorporated by expanding the temporal and spatial derivatives in the momentum equation, taking firstly the left-hand side of equation (8).

$$\mathrm{LHS} = \rho^l\frac{\partial}{\partial t}\left(g^l\vec{v}^l\right) + g^l\vec{v}^l\frac{\partial\rho\!\!\!/}{\partial t} + \vec{v}^l\nabla\cdot\left(\rho^l g^l \vec{v}^l\right) + \underline{\nabla}\vec{v}^l\left(\rho^l g^l \vec{v}^l\right) \tag{9a}$$

$$= \rho^l\underbrace{\frac{\partial}{\partial t}\left(g^l\vec{v}^l\right)}_{\substack{\text{Unsteady}\\\text{Acceleration}}} + \left(\rho^l - \rho^s\right)\underbrace{\frac{\partial g^s}{\partial t}\vec{v}^l}_{\substack{\text{Shrinkage}\\\text{Acceleration}}} + \rho^l\underbrace{\underline{\nabla}\vec{v}^l\left(g^l\vec{v}^l\right)}_{\substack{\text{Advective}\\\text{Acceleration}}} \tag{9b}$$

The development in (9b) shows that the origin of the flow, namely its acceleration, is attributed to three causes: i) unsteady acceleration: a temporal change of a particle's velocity, ii) shrinkage-induced acceleration: a local "suction" effect at the solid-liquid interface (where $\frac{\partial g^s}{\partial t} > 0$) caused by the density jump $\left(\rho^l - \rho^s\right)$ and iii) convective acceleration: a spatial change in the velocity field. The effect of the *shrinkage-induced* flow is introduced using the mass balance in equation (3). The right-hand side of equation (8) is now expanded:

$$\mathrm{RHS} = \vec{\nabla}\cdot\left(\langle p^l\rangle\underline{\mathbb{I}} + 2\mu^l\langle\underline{\dot{\varepsilon}}^l\rangle + \langle\underline{\tau}^l\rangle\right) + g^l\rho^l\vec{g} + \vec{\Gamma}^l_p + \vec{\Gamma}^l_{\mathbb{S}} \tag{10a}$$

$$= -\vec{\nabla}\left(g^l p^l\right) + \vec{\nabla}\cdot\left(2\mu^l\langle\underline{\dot{\varepsilon}}^l\rangle\right) + \vec{\nabla}\cdot\left(-\frac{2}{3}\mu^l\nabla\cdot\langle\vec{v}^l\rangle\underline{\mathbb{I}}\right) + g^l\rho^l\vec{g} + \vec{\Gamma}^l_p + \vec{\Gamma}^l_{\mathbb{S}} \tag{10b}$$

$$= -p^l\vec{\nabla}g^l\!\!\!\!\diagup - g^l\vec{\nabla}p^l + \vec{\nabla}\cdot\left(2\mu^l\langle\underline{\dot{\varepsilon}}^l\rangle\right) + \vec{\nabla}\cdot\left(-\frac{2}{3}\mu^l\nabla\cdot\langle\vec{v}^l\rangle\underline{\mathbb{I}}\right) + g^l\rho^l\vec{g} + \vec{\Gamma}^l_p\!\!\!\!\diagup + \vec{\Gamma}^l_{\mathbb{S}} \tag{10c}$$

$$= -g^l\vec{\nabla}p^l + \vec{\nabla}\cdot\left(\mu^l\left(\underline{\nabla}\langle\vec{v}^l\rangle + {}^{\mathbf{t}}\underline{\nabla}\langle\vec{v}^l\rangle\right)\right) + \vec{\nabla}\left(-\frac{2}{3}\mu^l\frac{\rho^l-\rho^s}{\rho^l}\frac{\partial g^s}{\partial t}\right) + g^l\rho^l\vec{g} - g^{l2}\mu^l\mathbb{K}^{-1}\vec{v}^l \tag{10d}$$

The system thus consists of 3 equations (one for each of the components of $\vec{v}^l$) and 4 unknowns ($\vec{v}^l_x$, $\vec{v}^l_y$, $\vec{v}^l_z$ and p). An additional equation is provided by the mass continuity equation (3). For convenience, the superficial velocity $\langle\vec{v}^l\rangle$ will be chosen as a velocity unknown instead of the intrinsic average: $\langle\vec{v}^l\rangle = g^l\vec{v}^l$. The final system to solve, after grouping the unknowns in the LHS and the remaining terms in the RHS, is given by:

$$\begin{cases} \rho^l \dfrac{\partial \langle \vec{v}^l \rangle}{\partial t} + \dfrac{\rho^l - \rho^s}{g^l} \dfrac{\partial g^s}{\partial t} \langle \vec{v}^l \rangle + \rho^l \underline{\nabla} \vec{v}^l \langle \vec{v}^l \rangle + \vec{\nabla} \cdot \left(2\mu^l \langle \underline{\dot{\varepsilon}}^l \rangle \right) + g^l \mu^l \mathbb{K}^{-1} \langle \vec{v}^l \rangle \\[3mm] \qquad = g^l \vec{\nabla} p^l + \vec{\nabla} \left(-\dfrac{2}{3} \mu^l \nabla \cdot \langle \vec{v}^l \rangle \right) + g^l \rho^l \vec{g} \\[3mm] \nabla \cdot \langle \vec{v}^l \rangle = \dfrac{\rho^l - \rho^s}{\rho^l} \dfrac{\partial g^s}{\partial t} \end{cases}$$

$$\tag{11}$$

4 Energy Conservation

We have seen the averaged energy conservation equation in the case of two phases: a solid phase and an incompressible liquid phase. However, with the incorporation of the shrinkage effect, new terms should appear in the advective-diffusive heat transfer equation.

4.1 Assumptions

- The thermal conductivity is constant for both phases: $\langle \kappa \rangle = \kappa^s = \kappa^l = \kappa$

- Consequence of the static solid phase: $\langle \rho h \vec{v} \rangle = g^l \rho^l h^l \vec{v}^l + g^s \rho^s h^s \vec{v}^s = g^l \rho^l h^l \vec{v}^l$

- The system's enthalpy may thermodynamically evolve with pressure, knowing that $h = e + \frac{p}{\rho}$, where e is the internal energy and p is the pressure. It infers that the heat transport equation may contain a contribution attributed to volume compression/expansion:

$$\frac{\partial p}{\partial t} + \nabla \cdot \left(p\vec{v} \right) = \frac{\partial p}{\partial t} + p\nabla \cdot \vec{v} + \vec{v} \cdot \vec{\nabla} p \tag{12}$$

  In the literature, this contribution has been always neglected, even when accounting for solidification shrinkage, owing to the small variations of pressure.

- Another contribution is also neglected in solidification problems, that is the heat generated by mechanical deformation, $\mathbb{S} : \dot{\varepsilon}$

4.2 Formulation

The unknowns in the energy conservation are the average volumetric enthalpy $\langle \rho h \rangle$ and temperature T. The energy conservation equation writes:

$$\frac{\partial \langle \rho h \rangle}{\partial t} + \nabla \cdot \langle \rho h \vec{v} \rangle = \nabla \cdot \left(\langle \kappa \rangle \vec{\nabla} T \right) \tag{13a}$$

$$\frac{\partial \langle \rho h \rangle}{\partial t} + \nabla \cdot \left(g^l \rho^l h^l \vec{v}^l \right) = \nabla \cdot \left(\kappa \vec{\nabla} T \right) \tag{13b}$$

$$\frac{\partial \langle \rho h \rangle}{\partial t} + \rho^l h^l \nabla \cdot \langle \vec{v}^l \rangle + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l h^l \right) = \nabla \cdot \left(\kappa \vec{\nabla} T \right) \tag{13c}$$

$$\frac{\partial \langle \rho h \rangle}{\partial t} + \cancel{\rho^l} h^l \frac{\rho^l - \rho^s}{\cancel{\rho^l}} \frac{\partial g^s}{\partial t} + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l h^l \right) = \nabla \cdot \left(\kappa \vec{\nabla} T \right) \tag{13d}$$

$$\frac{\partial \langle \rho h \rangle}{\partial t} + \left(\rho^l - \rho^s \right) h^l \frac{\partial g^s}{\partial t} + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l h^l \right) = \nabla \cdot \left(\kappa \vec{\nabla} T \right) \tag{13e}$$

$$\boxed{\frac{\partial \langle \rho h \rangle}{\partial t} + \rho^l \langle \vec{v}^l \rangle \cdot \vec{\nabla} h^l = \nabla \cdot \left(\kappa \vec{\nabla} T \right) + \left(\rho^s - \rho^l \right) h^l \frac{\partial g^s}{\partial t}} \tag{14}$$

4.3 Discussion

In order to keep things simple, the term "enthalpy" will refer henceforth to "volume enthalpy", otherwise, we will explicitly use the term "mass enthalpy". It is important to understand the meaning of the terms in equation (14). The first term in the left-hand side is the temporal change in the system's average enthalpy, i.e. a temporal change in the volume enthalpy of any of the phases in the course of solidification. The second LHS term is a dot product between the superficial liquid velocity and the the gradient of the liquid's enthalpy. Since phase densities are constant in our case, the gradient term reduces to the liquid's mass enthalpy. If we consider a representative volume element (RVE) in the liquid phase, far from the mushy zone, we can stipulate:

$$\vec{\nabla} h^l = C_p^l \vec{\nabla} T \tag{15}$$

assuming that the phase mass specific heat, C_p^l, is constant. Therefore, the liquid enthalpy is advected in the case where the velocity vector is not orthogonal to the temperatre gradient. The advection reaches its maximum when the two vectors have the same direction. Consider, for instance, a filled ingot with a cooling flux applied to its bottom surface. If the density variation with temperature were to be neglected, then the sole mechanical driving force in the melt is the density jump at the solid-liquid interface ahead of the mushy zone. The temperature gradient in such a case is vertical upward, while the velocity vector is in the opposite direction. The advective term writes:

$$\rho^l \langle \vec{v}^l \rangle \cdot \vec{\nabla} h^l = -\rho^l C_p^l \| \langle \vec{v}^l \rangle \| \| \vec{\nabla} T \| \tag{16}$$

We see that the second RHS term in equation (14) acts as a heat source at the interface between the the phases, in this particular solidification scenario. Another heat power (of unit $W m^{-3}$) adds to the system within the mushy, that is the second term in the right-hand side of the same equation. This term is proportional to the solidification rate. Finally, the first RHS term accounts for thermal diffusion within the phases.

It should be emphasized that the assumption of a constant specific heat in the

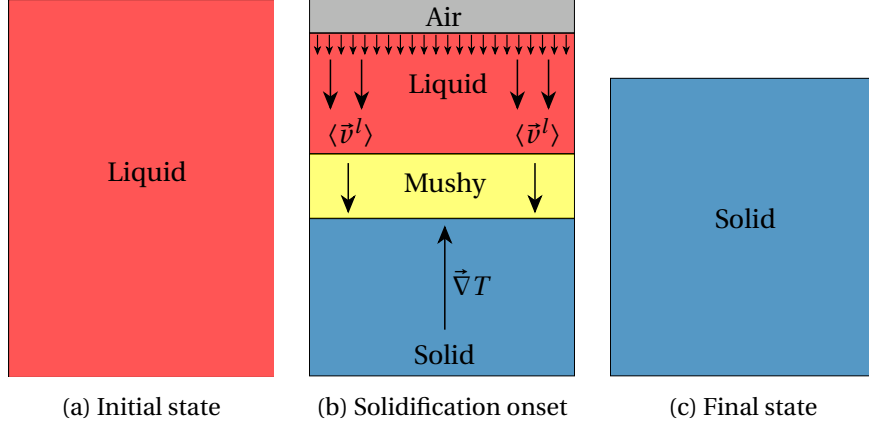(a) Initial state   (b) Solidification onset   (c) Final state

Figure 2: Effect of shrinkage flow on a solidifying ingot

liquid in equation (15) applies when no macrosegregation occurs. Nonetheless, when the latter is considered, the phases specific and latent heats become highly dependent on the local average composition. It then advisable to use the thermodynamic tabulation approach, where the enthalpies are directly tabulated as functions of temperature and composition.

5 Species Conservation

The last conservation principle is applied to the chemical species or solutes. This principle allows predicting macrosegregation when applied to a solidification system, along with the mass, momentum and energy balances. However, the conservation equation should be reformulated in the case of a melt flow driven by shrinkage.

5.1 Assumptions

- The alloy is binary, i.e., it is composed from one solute, and hence the notation of the average composition without a solute index: $\langle w \rangle$ for the mass composition and $\langle \rho w \rangle$ for the volume composition

- The solid fration is determined assuming complete mixing in both phases, hence the lever rule is applicable. It should be mentionned that the solidification path in the current approach is tabulated using thermodynamic data at equilibrium

- The solutal diffusion coefficient D^s in the solid phase is neglected in the mass diffusive flux term. The remaining term, D^l, is a mass diffusion coefficient in the liquid phase, of unit $m^2 s^{-1}$

- Consequence of the static solid phase: $\langle \rho w \vec{v} \rangle = g^l \rho^l \langle w \rangle^l \vec{v}^l + \cancel{g^s \rho^s \langle w \rangle^s \vec{v}^s} = g^l \rho^l \langle w \rangle^l \vec{v}^l$

5.2 Formulation

The species conservation is pretty similar the energy conservation formluted in the previous section. For a binary alloy, we can write:

$$\frac{\partial \langle \rho w \rangle}{\partial t} + \nabla \cdot \langle \rho w \vec{v} \rangle = \nabla \cdot \left(\rho^l \langle D^l \rangle \vec{\nabla} \langle w \rangle^l \right) \tag{17a}$$

$$\frac{\partial \langle \rho w \rangle}{\partial t} + \nabla \cdot \left(g^l \rho^l \langle w \rangle^l \vec{v}^l \right) = \nabla \cdot \left(g^l \rho^l D^l \nabla \langle w \rangle^l \right) \tag{17b}$$

$$\frac{\partial \langle \rho w \rangle}{\partial t} + \rho^l \langle w \rangle^l \nabla \cdot \langle \vec{v}^l \rangle + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l \langle w \rangle^l \right) = \nabla \cdot \left(g^l \rho^l D^l \vec{\nabla} \langle w \rangle^l \right) \tag{17c}$$

$$\frac{\partial \langle \rho w \rangle}{\partial t} + \rho^l \langle w \rangle^l \frac{\rho^l - \rho^s}{\rho^l} \frac{\partial g^s}{\partial t} + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l \langle w \rangle^l \right) = \nabla \cdot \left(g^l \rho^l D^l \vec{\nabla} \langle w \rangle^l \right) \tag{17d}$$

$$\frac{\partial \langle \rho w \rangle}{\partial t} + \left(\rho^l - \rho^s \right) \langle w \rangle^l \frac{\partial g^s}{\partial t} + \langle \vec{v}^l \rangle \cdot \vec{\nabla} \left(\rho^l \langle w \rangle^l \right) = \nabla \cdot \left(g^l \rho^l D^l \vec{\nabla} \langle w \rangle^l \right) \tag{17e}$$

$$\boxed{\frac{\partial \langle \rho w \rangle}{\partial t} + \rho^l \langle \vec{v}^l \rangle \cdot \vec{\nabla} \langle w \rangle^l = \nabla \cdot \left(\rho^l D^l \vec{\nabla} \langle w \rangle^l \right) + \left(\rho^s - \rho^l \right) \langle w \rangle^l \frac{\partial g^s}{\partial t}} \tag{18}$$

5.3 Discussion

The species transport equation is usually derived with the volumetric average composition $\langle \rho w \rangle$, then divided by the density, which is constant if no solidification shrinkage occurs. In the case where macrosegregation is solely due to fluid flow generated by natural or forced convection, the overall volume remains constant. It is thus convenient to compute composition variations using the mass variable $\langle w \rangle$. However, in the current context, the volume is subject to changes, hence the formulation of equation (18) with $\langle \rho w \rangle$.