



## Towards wall functions for the prediction of solute segregation in plane front directional solidification



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### ABSTRACT

The present paper focuses on solute segregation occurring in directional solidification processes with sharp solid/liquid interface, like silicon crystal growth. A major difficulty for the simulation of such processes is their inherently multi-scale nature: the impurity segregation problem is controlled at the solute boundary layer scale (micrometers) while the thermal problem is ruled at the crucible scale (meters). The thickness of the solute boundary layer is controlled by the convection regime and requires a specific refinement of the mesh of numerical models. In order to improve numerical simulations, wall functions describing solute boundary layers for convecto-diffusive regimes are derived from a scaling analysis. The aim of these wall functions is to obtain segregation profiles from purely thermo-hydrodynamic simulations, which do not require solute boundary layer refinement at the solid/liquid interface. Regarding industrial applications, various stirring techniques can be used to enhance segregation, leading to fully turbulent flows in the melt. In this context, the scaling analysis is further improved by taking into account the turbulent solute transport. The solute boundary layers predicted by the analytical model are compared to those obtained by transient segregation simulations in a canonical 2D lid driven cavity configuration for validation purposes. Convective regimes ranging from laminar to fully turbulent are considered. Growth rate and molecular diffusivity influences are also investigated. Then, a procedure to predict concentration fields in the solid phase from a hydrodynamic simulation of the solidification process is proposed. This procedure is based on the analytical wall functions and on solute mass conservation. It only uses wall shear-stress profiles at the solidification front as input data. The 2D analytical concentration fields are directly compared to the results of the complete simulation of segregation in the lid driven cavity configuration. Finally, an additional output from the analytical model is also presented. We put in light the correlation between different species convecto-diffusive behaviour; we use it to propose an estimation method for the segregation parameters of various chemical species knowing segregation parameters of one specific species.

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### 1. Introduction

The present work is related to solidification from the melt processes with sharp solid/liquid interface, like silicon crystal growth. In such processes solute segregation represents an important issue regarding material quality. For instance, in the field of photovoltaic silicon production, the control of dopant concentrations and the

removal of metallic impurities are important parameters regarding solar cells efficiency [1–3]. The numerical simulation of heat, momentum and solute transport in the melt is a powerful tool for process optimizations [4–6]. Nevertheless, the variety of involved length scales is a drawback for the study of industrial configurations. First of all, a precise description of the furnace thermal conditions is mandatory for a realistic description of the crystallization process, including growth rate variations and interface curvature. Heat transfers between the main components of the furnace must be computed, resulting in characteristic dimensions in the range of meters for industrial scale furnaces [7–9]. On the other hand, the description of the solute boundary layer at the

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solidification front requires a very thin discretization. For silicon crystal growth under natural convection, the solute boundary layer thickness is in the order of 1 mm (assuming a molecular diffusivity  $D \sim 10^{-8} \text{ m}^2/\text{s}$  and an interface velocity  $V_I \sim 10 \text{ } \mu\text{m}/\text{s}$ ). The use of stirring systems to enhance segregation leads to even thinner solute boundary layers with possibly fully turbulent flows [10–14]. Therefore, there is a real interest in the development of coupled methods, with heat and momentum transport simulations on one side and solute transport scaling analysis on the other side. This simplification of the problem remains reasonable as far as dilute alloys are concerned, solute concentrations remaining sufficiently low to have negligible influence on heat and momentum transport.

In their fundamental work on solute segregation, Burton et al. [15] have established that a key parameter of the segregation problem is the thickness of the solute boundary layer at the solid/liquid interface, which is controlled by molecular diffusion and convective transport in the melt. A definition of the solute boundary layer thickness  $\delta$  has been proposed by Wilson [16]. This definition proved to be an efficient way to determine the effective segregation coefficient  $k_{\text{eff}}$  from a convecto-diffusive parameter  $\Delta$ . Recently, Garandet et al. [17] introduced an analytical model of the solute boundary layer. This model is derived from a scaling analysis of the solute transport equation and predicts the convecto-diffusive parameter from the wall shear-stress at the solid/liquid interface. In their study, a steady-state 2D lid driven cavity configuration is used as a reference case for segregation under various convective regimes. Then, Kaddeche et al. [18] tested this model on an horizontal *Bridgman* configuration and compared it with experimental and numerical results. Both studies highlight the ability of the model to predict the mean segregation regime from an averaged value of the wall shear-stress obtained from a hydrodynamic simulation of the melt convection flow. This model was also tested in a transient regime with a 2D lid driven cavity flow [19]. This study shows that the analytical model provides a good estimate of the lateral segregations using local values of wall shear-stress at the solid/liquid interface. The model can also describe transient variations of the segregation regime for low frequency perturbations of the convection regime and solidification rate, in the limits of the quasi-steady assumption used for the scaling analysis of the solute boundary layer.

The aim of this paper is to demonstrate that an analytical formulation of the solute boundary layer, derived from a scaling analysis, can provide a meaningful description of segregations occurring in directional solidification processes. This approach leads to the definition of solute wall functions describing solute boundary layers for convecto-diffusive regimes, up to fully turbulent flows. Section 2 is dedicated to the formulation and validation of such solute wall functions. The original model proposed by Garandet et al. [17] is revised, in order to account for turbulent transport inside the solute boundary layer. Solute boundary layers obtained from these wall functions are compared to numerical results of segregation in the transient lid driven cavity configuration, which proved to be a meaningful parametric reference case [19]. In Section 3, the developed analytical model is used to retrieve segregation profiles from hydrodynamic simulations. An iterative procedure based on solute mass conservation is proposed to access solute repartition in the solid. This procedure is applied to the 2D lid driven cavity configuration and the analytical concentration fields are directly compared to those obtained numerically. Finally, Section 4 presents an application of the model for the study of different species segregation. A correlation between the segregation parameters of the different species is derived from the solute boundary layer model.

## 2. Turbulent transport in solute boundary layers

### 2.1. Solute boundary layer analytical model

We consider a quasi 1D directional solidification process. A weakly concentrated liquid metallic blend or semiconductor is progressively solidified. The plane solidification front progresses in the  $z$  direction. Let us recall that a jump in impurity (or solute) concentration at the solid/liquid interface is imposed between concentrations on the liquid side,  $C_L^l$ , and the solid side,  $C_S^l$ , since the impurity solubility is different in these two phases. Very often a smaller solubility is observed in the solid than in the liquid, leading to a thermodynamic segregation coefficient,  $k_0 = C_S^l/C_L^l$ , smaller than one. The consequence is that, while the solidification progresses, solute is rejected from the solid phase towards the liquid phase, which leads to the formation of a solute boundary layer in the liquid in the vicinity of the front. Burton et al. [15] explain that solute incorporation in the solid depends on the solute boundary layer at the solidification front. Wilson [16] proposed the following definition of the solute boundary layer thickness:

$$\delta = \frac{C_L^l - C_L^\infty}{-(\partial C_L / \partial z)_I}, \quad (1)$$

where  $C_L^l$  and  $C_L^\infty$  stand for solute mass fraction in the liquid at the solid/liquid interface and outside the solute boundary layer, respectively. Assuming negligible diffusion in the solid, solute conservation at the interface is given by:

$$-D \frac{\partial C_L}{\partial z} \Big|_I = V_I (1 - k_0) C_L^l, \quad (2)$$

with  $D$  the solute molecular diffusivity in the liquid ( $\text{m}^2/\text{s}$ ),  $V_I$  the interface velocity ( $\text{m}/\text{s}$ ) and  $k_0$  the thermodynamic segregation coefficient. The effective segregation coefficient is then defined by:

$$k_{\text{eff}} = \frac{k_0 C_L^l}{C_L^\infty} = \frac{k_0}{1 - (1 - k_0) \Delta}, \quad (3)$$

where the convecto-diffusive parameter  $\Delta$  represents the normalized solute boundary layer thickness:

$$\Delta = \frac{\delta V_I}{D} = \frac{C_L^l - C_L^\infty}{C_L^l (1 - k_0)}, \quad (4)$$

since the solute boundary layer thickness for a purely diffusive regime is given by the ratio  $D/V_I$ .

The analytical model proposed by Garandet et al. [17] describes the solute boundary layer in convecto-diffusive regimes. It is derived from a scaling analysis of the solute transport equation in the liquid phase. At first, the analysis was presented for the lid-driven cavity configuration, but it can easily be transposed to other configurations. We shall consider here the general case of a boundary layer flow developing over a plane solidification front. This configuration is presented in Fig. 1. A boundary-layer flow develops over the solid/liquid interface, from an impingement point (on the right side) to a separation point (on the left side). The characteristic length over which the boundary layer flow takes place is denoted  $l_c$ , and the vertical velocity gradient at the interface leads to a wall shear-stress  $\tau = \mu(\partial u / \partial z)_{z=0}$ , with  $u$  the velocity component parallel to the interface ( $\text{m}/\text{s}$ ) and  $\mu$  the liquid dynamic viscosity ( $\text{Pa s}$ ).

As explained in former studies [17,20], the scaling analysis of the solute transport equation leads to a simplified equation for  $\delta$ :

$$\frac{D}{\delta} = V_I - w(\delta), \quad (5)$$

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