

# Solute segregation in a lid driven cavity: Effect of the flow on the boundary layer thickness and solute segregation

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## ABSTRACT

Our objective in the present work is to study the effect of convective flows, ranging from laminar to fully turbulent, on solute segregation in directional solidification configurations. To do so, numerical simulations performed in a model 2D lid driven cavity; the problem parameters, apart from the species molecular diffusion coefficient, are the lid and growth velocities. Purely diffusive to fully convective mass transport conditions are modelled in our parametric study. In parallel, a scaling analysis aiming at the determination of the solute boundary layer thickness is proposed. The results show that a single non-dimensional number, based on the interface stress, is able to capture the physics of the solute transport phenomena.

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## 1. Introduction

Heat and solute transfer issues are of paramount importance for the control of the crystal growth of semiconductors and metals from the liquid phase, and specially so in the case of Si crystals with applications in the microelectronic and photovoltaic industries, see e.g. [1–3]. In crucible of large dimensions, convection often dominates solute transport, due to the generally low values of the Fickian diffusion coefficients. As a consequence, a number of techniques have been proposed in recent years in order to tailor fluid flows in the melt. Among them, and without any claim to exhaustivity, one can think of travelling [3–5], alternating [6,7], rotating [8] or mixed [9] magnetic fields, as well as crucible vibration [10], acoustic streaming [11].

One application of interest for industrial purposes, that of the purification of metallurgical grade silicon by directional solidification, relies on the fact that most metals have very low partition coefficients in Si [12]. Therefore, an efficient solute segregation is in principle possible, provided of course that the process parameters are selected to ensure that the effective and thermodynamic partition coefficients remain close to each other [13]. Since high interface velocities are known to lead to effective partition coefficients approaching unity (see e.g. [14–16]), the development

of efficient stirring systems is a necessity to guarantee an adequate process productivity.

The purpose of the present paper is to propose a coupled numerical modelling scaling analysis approach to identify the requirements in terms of convective flow in order to ensure that the effective partition coefficient remains small even at high growth velocities. To do so, rather than aiming at the accurate description of a given experimental configuration, we will focus on the model problem of convective and species transport in a two dimensional domain with a moving boundary opposite to the crystal growth interface, i.e. in the so-called “lid driven” cavity flow [17,18].

It should be kept in mind that, in spite of its relatively ancient nature, the lid driven cavity problem is still a topic of debate, even at relatively modest Reynolds number. A feature of the targeted application of metallurgical grade silicon purification is that both the melt dimensions and the stirring velocities are expected to be quite large, say at least 20 cm and 10 cm/s, respectively. With such typical values, the flow field within the cavity is expected to be fully turbulent for a fluid like silicon that like most metals has a low kinematic viscosity. Nevertheless, our simulations will cover both laminar and turbulent flows.

The choice of focusing on an idealised 2D configuration without considering the coupling with heat transfer phenomena allows to perform a large number of numerical simulations. The main parameters are the lid and interface velocities, as well as the species diffusion coefficients, which, even in a material as widely

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studied as silicon, remain subject to large uncertainties [19,20]. The results are presented in terms of the convecto-diffusive parameter [15,16], which can be easily related to the effective partition coefficient (see Section 2 below), and has the advantage of being amenable to a scaling analysis.

Regarding the organisation of the manuscript, Section 2 will be devoted to a presentation of the problem formulation in mathematical terms, as well as to some basics on solute segregation. We shall then in Section 3 focus on the numerical technique and results, before turning in Section 4 to the scaling analysis that allows to identify the relevant parameters of the solute transport problem.

## 2. Background on solute segregation and problem formulation

It appears interesting at this point to recall some basic ideas on segregation phenomena. Among the pioneering papers on the topic, a special mention should be made of the work of Burton, Prim and Schlichter [14], who were the first to understand the key role played by the solute rich region ahead of the growth interface. Later on, Wilson [15] proposed a physically sound definition of this solutal boundary layer thickness  $\delta$ :

$$\delta = -(C_l - C_\infty) / (dC/dZ)_l \quad (1)$$

with  $C_l$  and  $C_\infty$  denoting the composition levels, respectively, at and far away from the growth interface. The  $Z$ -axis points normal to that interface in the direction of the bulk liquid (see Fig. 1). In parallel, solute conservation at the solidification front can be expressed as:

$$-D(dC/dZ)_l = V_l(1-k)C_l \quad (2)$$

In the above equation,  $D$ ,  $V_l$  and  $k$ , respectively, stand for the species molecular diffusivity, the growth velocity and the thermodynamic partition coefficient as given by the phase diagram of the Si-impurity system. Combining Eqs. (1) and (2), one gets an expression for the effective partition coefficient:

$$k_{eff} = kC_l/C_\infty = k / (1 - (1-k)\Delta) \quad (3)$$

$\Delta = \delta V_l / D$  being a convecto-diffusive parameter whose value ranges from 0 for the case of intense fluid flow in the fluid (corresponding to a melt of virtually uniform composition) to one in purely diffusive solute transport conditions. The control of

impurity segregation is thus reduced to the determination of the convecto-diffusive parameter  $\Delta$  as a function of the process and thermophysical parameters of the problem, namely in our present case the lid and interface velocities along with the diffusion coefficient.

The existence of a well defined range for the variation of the solute composition ahead of the growth interface allows a further simplification by the use of order of magnitude, or scaling analyses [21]. Assuming the time variations to be slow (quasi steady-state approximation) and the gradients associated to composition variations parallel to the interface to be negligible, one can find a simple relation between the solutal boundary layer thickness, the growth rate and the convection velocity normal to the interface, taken at the boundary layer scale,  $W(\delta)$  [22]:

$$D/\delta = V_l - W(\delta). \quad (4)$$

For conditions where the flow in the melt can be considered laminar, the predictions of Eq. (4) were found to be in satisfying agreement with existing numerical [22,23] and experimental [24] data.

It is one of the objectives of the present work to show that Eq. (4) can also be used in the case of fully turbulent flow, but this requires the construction of an adequate velocity profile in the vicinity of the growth interface to estimate  $W(\delta)$ . This will be done in Section 4, but we first have to present in more detail our model problem and the numerical procedure. In our 2D square cavity (see also Fig. 1 for a set of notations), momentum and species conservation in the melt can be expressed by the classical Navier–Stokes and Fick equations, written here as:

$$\partial V/\partial t + (V \cdot \nabla)V = -\nabla P/\rho + \nu \nabla^2 V \quad (5)$$

$$\partial C/\partial t + (V \cdot \nabla)C = D \nabla^2 C \quad (6)$$

In the above equations,  $V$ ,  $P$ ,  $C$ ,  $\rho$  and  $\nu$ , respectively, stand for the velocity, pressure and composition fields, the volumic mass and the kinematic viscosity of the fluid. The solid liquid interface is defined as  $Z=0$ . This amounts to assuming that the Prandtl number of the fluid is essentially zero, which means that the interface will not be deformed by motion of the fluid.

From a physical standpoint, in a frame moving with the interface, the boundary conditions can be expressed as:

Solid–liquid front ( $Z=0$ ,  $0 \leq X \leq H$ ):

$$V = 0 \quad (7a)$$

$$-D(\partial C/\partial Z)_l = V_l(1-k)C_l \quad (7b)$$

Lateral walls ( $X=0$ ,  $0 \leq Z \leq H$  and  $X=H$ ,  $0 \leq Z \leq H$ ):

$$V = 0 \quad (8a)$$

$$\partial C/\partial X = 0 \quad (8b)$$

Top wall ( $Z=H$ ,  $0 \leq X \leq H$ ):

$$V = V_l e_x \quad (9a)$$

$$C = C_0 \quad (9b)$$

In Eqs. (9a) and (9b),  $V_l$  and  $C_0$ , respectively, stand for the lid velocity and a reference concentration.

Since we consider only dilute alloys (even in metallurgical grade Si the total impurity content rarely exceeds 1%), the volumic mass and the kinematic viscosity of the fluid will be taken equal to those of pure silicon, namely  $\rho = 2.55 \times 10^3 \text{ kg/m}^3$  [25],  $\nu = 3.5 \times 10^{-7} \text{ m}^2/\text{s}$  [26,27]. On the other hand, the species diffusion coefficient will be taken as a problem parameter, since, in addition to the intrinsic uncertainties mentioned earlier, we are interested in the segregation of all possible impurities. At this

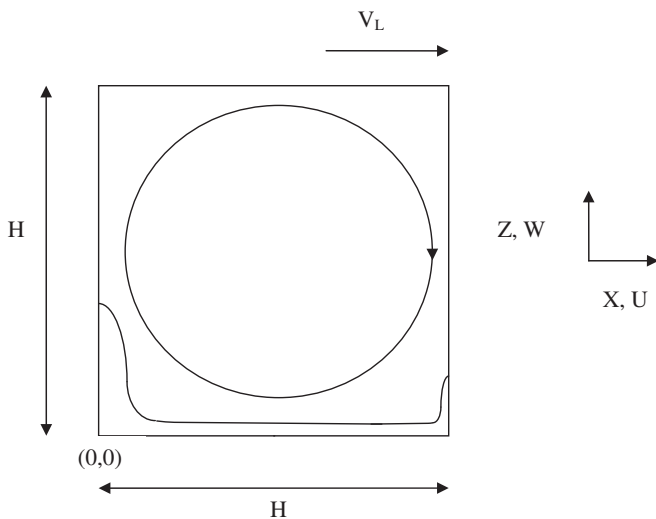


Fig. 1. Problem geometry and coordinate axes. Schematic iso-stream function and iso-concentration lines are also shown.

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