Modelling of 3D Melt Flow in Czochralski Crystal Growth

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Abstract. This paper is devoted to the numerical solution of a stationary three–dimensional model consisting of the Boussinesq approximation of the Navier–Stokes equations coupled with two convection–diffusion equations. The problem is complicated by nonstandard boundary conditions for velocity on the liquid–gas interface where tangential surface forces proportional to surface gradients of temperature and concentration (Marangoni effect) and zero normal component of the velocity are supposed. The discretization of the problem is performed using a finite element method based on tetrahedral triangulations approximating the computational domain. For high Reynolds numbers, a special kind of stabilization is employed. Results on existence and convergence of the discrete solutions are stated under general assumptions, numerical solution of the discrete problem is explained and some numerical results are presented.

Keywords: Navier–Stokes equations, Boussinesq aproximation, Czochralski method, nonstandard boundary conditions, finite element method, numerical simulation

Mathematics Subject Classification (MSC 1991): 76D05, 76Rxx, 65N30

1 Formulation of the Problem

The Czochralski method (cf. e.g. [1] or [6]) is the mostly used technique for producing semiconductor single crystals, the most important of which are silicon crystals. The semiconductor crystals are the basis materials for manufacturing various semiconductor devices like transistors, thyristors, integrated circuits, diodes etc. The quality of the crystals produced by the Czochralski method can be influenced by many parameters and since direct measurements of effects caused by various combinations of these parameters are very difficult, mathematical modelling and numerical simulations of the Czochralski method are necessary.

The main feature of the Czochralski method is that the grown single crystal is pulled from its melt which is situated in a crucible (cf. Fig. 1). The device is rotationally symmetrical and, during the pulling, both the crucible and the crystal perform rotational motions around the symmetry axis and, at the same time, motions in the vertical direction which correspond to the crystal growth velocity and maintain the melt free surface in a constant position. The crystal growth velocity is usually considerably smaller than the typical velocities in the melt. Crucible for growing silicon crystals are made of vitreous silica which leads to a contamination of the melt by oxygen.

The problem considered in this paper is a stationary three–dimensional mathematical model describing the processes in the melt during a silicon single crystal pulling

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by the Czochralski method. The region occupied by the melt is assumed to be known a priori and will be denoted by Ω in the following. The boundary of Ω comprises the crucible wall Γ^W, the melt free surface Γ^{LG} and the interface Γ^{LS} between the melt and the growing crystal (cf. Fig. 1). We assume that $\Omega \subset \mathbb{R}^3$ is a bounded domain with a Lipschitz–continuous boundary $\partial\Omega$ and that the sets Γ^W, Γ^{LG} and Γ^{LS} are open in $\partial\Omega$, disjoint and have positive measures. In addition, we suppose that there exists an extension $\boldsymbol{m} \in W^{1,4}(\Omega)^3$ of the unit outward normal vector to Γ^{LG}, i.e., $\boldsymbol{m}|_{\Gamma^{LG}} = \boldsymbol{n}|_{\Gamma^{LG}}$. This assumption is satisfied e.g. if both Γ^{LG} and $\partial\Gamma^{LG}$ are sufficiently regular.

The mathematical model consists of four coupled partial differential equations, which can be derived from general balance laws for linear momentum, mass, energy, and mass of a constituent, respectively, and of the corresponding boundary conditions:

$$\left.\begin{aligned}
&-\Delta\,\boldsymbol{v} + \alpha_5\,(\nabla\,\boldsymbol{v})\boldsymbol{v} + \alpha_5\,\nabla\,p = \alpha_1\,\boldsymbol{f}_1(\theta) + \alpha_2\,\boldsymbol{f}_2(c)\,, && (1.1)\\
&\operatorname{div}\boldsymbol{v} = 0\,, && (1.2)\\
&-\Delta\,\theta + \alpha_6\,\boldsymbol{v}\cdot\nabla\,\theta = 0\,, && (1.3)\\
&-\Delta\,c + \alpha_7\,\boldsymbol{v}\cdot\nabla\,c = 0\,, && (1.4)
\end{aligned}\right\}\quad \text{in } \Omega$$

$$\boldsymbol{v} = \boldsymbol{v}_b\,, \qquad \theta = \theta_b\,, \qquad c = c_b \qquad \text{on } \Gamma^W, \tag{1.5}$$

$$\left.\begin{aligned}
&(\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n})(\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^{\mathrm{T}})\,\boldsymbol{n} = -\alpha_3\,\nabla_s\,\theta - \alpha_4\,\nabla_s\,c\,, && (1.6)\\
&\boldsymbol{v}\cdot\boldsymbol{n} = 0\,, \qquad -\frac{\partial\theta}{\partial\boldsymbol{n}} = \varphi_1(\theta)\,, \qquad c = c_b\,, && (1.7)
\end{aligned}\right\}\quad \text{on } \Gamma^{LG}$$

$$\boldsymbol{v} = \boldsymbol{v}_b\,, \qquad \theta = \theta_b\,, \qquad -\frac{\partial c}{\partial\boldsymbol{n}} = (\boldsymbol{v}_b\cdot\boldsymbol{n})\,\varphi_2(c) \qquad \text{on } \Gamma^{LS}. \tag{1.8}$$

We use the following notations: $\boldsymbol{v}$ is the velocity, p is the pressure, θ is the temperature, c is the oxygen concentration, $\boldsymbol{I}$ is the identity tensor, $\boldsymbol{n}$ is the unit outward normal vector to $\partial\Omega$, and ∇_s denotes the surface gradient (in this paper, $\nabla_s\,\cdot = (\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n})\,(\nabla\cdot)|_{\partial\Omega}$). The data of the model are assumed to satisfy the following assumptions:

$$\alpha_1, \alpha_2, \ldots, \alpha_7 \in \mathbb{R}^+\,, \tag{1.9}$$

$$\boldsymbol{f}_1, \boldsymbol{f}_2 \in C^1(\mathbb{R})^3, \quad |\boldsymbol{f}_1{}'(x)| \le 1, \quad |\boldsymbol{f}_2{}'(x)| \le 1 \quad \forall\, x \in \mathbb{R}\,, \tag{1.10}$$

$$\varphi_1, \varphi_2 \in C^1(\mathbb{R})\,, \tag{1.11}$$

$$\exists\; K_1,\, L_1 : \quad |\varphi_1(x)| \le K_1\,, \quad |\varphi_1{}'(x)| \le L_1 \quad \forall\, x \in \mathbb{R}\,, \tag{1.12}$$

$$\exists\; K_2,\, L_2 : \quad |\varphi_2(x)| \le K_2\,, \quad |\varphi_2{}'(x)| \le L_2 \quad \forall\, x \in \mathbb{R}\,, \tag{1.13}$$

$$\boldsymbol{v}_b \in H^{\frac{1}{2}}(\partial\Omega)^3\,, \quad \theta_b \in H^{\frac{1}{2}}(\partial\Omega)\,, \quad c_b \in H^{\frac{1}{2}}(\partial\Omega)\,, \tag{1.14}$$

$$\boldsymbol{v}_b\cdot\boldsymbol{n} = 0 \text{ on } \Gamma^{LG}, \quad \boldsymbol{v}_b\cdot\boldsymbol{n} \ge 0 \text{ on } \Gamma^{LS}, \quad \int_{\partial\Omega} \boldsymbol{v}_b\cdot\boldsymbol{n}\,\mathrm{d}\sigma = 0\,. \tag{1.15}$$

The equations (1.1) and (1.2) represent the Boussinesq approximation of the Navier–Stokes equations. Among the boundary conditions, the most interesting one is the

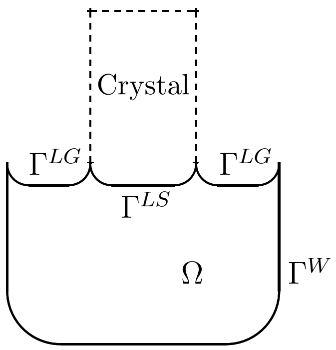

Figure 1 Cross–section through the melt and crystal in a Czochralski apparatus.

boundary condition (1.6) describing the so–called Marangoni effect, i.e. the fact that surface tension variations due to temperature and concentration gradients induce tangential surface forces on the melt free surface. The condition $\boldsymbol{v}_b \cdot \boldsymbol{n} \geq 0$ on Γ^{LS} is a natural condition which expresses that the crystal is really growing and not melting. From the physical point of view, the assumptions (1.9)–(1.15) do not present any loss of generality (cf. Remark 1.1). A detailed derivation and explanation of the model (1.1)–(1.8) can be found in [4].

Remark 1.1 The constants $\alpha_1, \ldots, \alpha_7$ have the following physical meanings:

$$\alpha_1 = \frac{Gr_\theta}{Re}\,, \quad \alpha_2 = \frac{Gr_c}{Re}\,, \quad \alpha_3 = \frac{Ma_\theta}{Re\,Pr}\,, \quad \alpha_4 = \frac{Ma_c}{Re\,Pr}\,, \quad \alpha_5 = Re\,, \quad \alpha_6 = Re\,Pr$$

and $\alpha_7 = Re\,Sc$, where Re is the Reynolds number, Pr is the Prandtl number, Sc is the Schmidt number, Gr is the Grashof number and Ma is the Marangoni number. The usual definitions of the functions $\boldsymbol{f}_1$, $\boldsymbol{f}_2$, φ_1, φ_2 are $\boldsymbol{f}_1(\theta) = -\theta\,\boldsymbol{e}_g$, $\boldsymbol{f}_2(c) = -c\,\boldsymbol{e}_g$ and

$$\varphi_1(\theta) = Bi\,(\theta - \theta_{amb}) + Rd\left\{(\theta + \widetilde{\theta})^4 - (\theta_{inf} + \widetilde{\theta})^4\right\}\,, \qquad \varphi_2(c) = Re\,Sc\,(k_0 - 1)\,(c + \widetilde{c})$$

for θ and c belonging to some *bounded* intervals (θ_1, θ_2) and (c_1, c_2), respectively. Outside these bounded intervals, the functions $\boldsymbol{f}_1$, $\boldsymbol{f}_2$, φ_1, φ_2 have no physical meaning and can be defined arbitrarily. In the above relations, $\boldsymbol{e}_g$ is a unit vector in the direction of the gravity, Bi is the Biot number, Rd is the radiation number, and k_0 is the segregation coefficient.

The plan of the paper is as follows. In Section 2, we establish a weak formulation of the problem (1.1)–(1.8) and mention some related results. Section 3 is devoted to the finite element discretization of the problem and, finally, in Section 4, we explain how the discrete problems can be solved numerically and present a few numerical results. The notation used in this paper is standard and can be found e.g. in [3]. We only mention that $\|\cdot\|_{k,p,\Omega}$ (resp. $|\cdot|_{k,p,\Omega}$) is the norm (resp. seminorm) in the Sobolev space $W^{k,p}(\Omega)$, $k = 0, 1, \ldots$, $p \in \langle 1, \infty\rangle$. For $p = 2$, the second index is dropped (i.e., we write $\|\cdot\|_{k,\Omega}$, resp. $|\cdot|_{k,\Omega}$) and the Sobolev space is denoted by $H^k(\Omega)$. The space of functions $v \in L^2(\Omega)$ satisfying $\int_\Omega v\,\mathrm{d}x = 0$ is denoted by $L^2_0(\Omega)$.

2 Weak Formulation and Its Solvability

In this section we establish a weak formulation of the problem (1.1)–(1.8) and state results on existence and uniqueness of the weak solutions. Details can be found in [4].

Before defining a weak formulation of (1.1)–(1.8), let us introduce the following notation:

$$
\begin{aligned}
&\widehat{\mathbf{W}} = \{\boldsymbol{v} \in H^1(\Omega)^3 \mid \boldsymbol{v}\cdot\boldsymbol{n} = 0 \ \text{ on } \Gamma^{LG}\}\,, \quad \mathbf{W} = \{\boldsymbol{v} \in \widehat{\mathbf{W}} \mid \boldsymbol{v} = \mathbf{0} \ \text{ on } \Gamma^W \cup \Gamma^{LS}\}\,,\\
&\Theta \ = \{\theta \in H^1(\Omega) \mid \theta = 0 \ \text{ on } \Gamma^W \cup \Gamma^{LS}\}\,, \quad \mathcal{C} \ = \{c \in H^1(\Omega) \mid c = 0 \ \text{ on } \Gamma^W \cup \Gamma^{LG}\}\,,\\
&a_1(\boldsymbol{v},\boldsymbol{w}) = \frac{1}{2}\int_\Omega (\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^{\mathrm{T}})\cdot(\nabla\boldsymbol{w} + \nabla\boldsymbol{w}^{\mathrm{T}})\,\mathrm{d}x\,, \qquad a_2(\theta,\eta) = \int_\Omega \nabla\theta\cdot\nabla\eta\,\mathrm{d}x\,,\\
&b_1(\boldsymbol{u},\boldsymbol{v},\boldsymbol{w}) = \int_\Omega \boldsymbol{w}\cdot(\nabla\boldsymbol{v})\boldsymbol{u}\,\mathrm{d}x\,, \qquad b_2(\boldsymbol{v},\theta,\eta) = \int_\Omega \eta\,\boldsymbol{v}\cdot\nabla\theta\,\mathrm{d}x\,,\\
&b(\boldsymbol{v},\lambda) = -\int_\Omega \lambda\,\mathrm{div}\,\boldsymbol{v}\,\mathrm{d}x\,,\\
&d(\zeta,\boldsymbol{w}) = \int_\Omega \nabla\zeta\cdot[\,\boldsymbol{w}\,\mathrm{div}\,\boldsymbol{m} - \boldsymbol{m}\,\mathrm{div}\,\boldsymbol{w} + (\nabla\boldsymbol{w})\,\boldsymbol{m} - (\nabla\boldsymbol{m})\,\boldsymbol{w}]\,\mathrm{d}x\,,\\
&<\mathrm{F}_1(\theta),\boldsymbol{w}> = \int_\Omega \boldsymbol{w}\cdot\boldsymbol{f}_1(\theta)\,\mathrm{d}x\,, \qquad <\mathrm{F}_2(c),\boldsymbol{w}> = \int_\Omega \boldsymbol{w}\cdot\boldsymbol{f}_2(c)\,\mathrm{d}x\,,\\
&<\Phi_1(\theta),\eta> = -\int_{\Gamma^{LG}} \eta\,\varphi_1(\theta)\,\mathrm{d}\sigma\,, \qquad <\Phi_2(c),\boldsymbol{\xi}> = -\int_{\Gamma^{LS}} (\boldsymbol{\xi}\cdot\boldsymbol{n})\,\varphi_2(c)\,\mathrm{d}\sigma\,,
\end{aligned}
$$

where $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{w} \in H^1(\Omega)^3$, c, θ, η, $\zeta \in H^1(\Omega)$, $\lambda \in L^2(\Omega)$ and $\boldsymbol{\xi} \in L^2(\partial\Omega)^3$. The bilinear form d is a generalization of the surface gradient on Γ^{LG} for functions from $H^1(\Omega)$ in the sense that

$$
d(\zeta,\boldsymbol{w}) = \int_{\Gamma^{LG}} \boldsymbol{w}\cdot\nabla_s\,\zeta\,\mathrm{d}\sigma \qquad \forall\ \zeta \in H^2(\Omega)\,,\ \ \boldsymbol{w} \in H^1(\Omega)^3,\ \boldsymbol{w}|_{\Gamma^W\cup\Gamma^{LS}} = \mathbf{0}\,.
$$

The form d does not depend on the choice of the extension $\boldsymbol{m}$ and vanishes for $\boldsymbol{w} \in H^1_0(\Omega)^3$.

Definition 2.1 Let $\widetilde{\boldsymbol{v}}_b \in H^1(\Omega)^3$, $\widetilde{\theta}_b$, $\widetilde{c}_b \in H^1(\Omega)$ be arbitrary functions satisfying

$$
\widetilde{\boldsymbol{v}}_b|_{\Gamma^W\cup\Gamma^{LS}} = \boldsymbol{v}_b\,, \quad \widetilde{\boldsymbol{v}}_b\cdot\boldsymbol{n}|_{\Gamma^{LG}} = 0\,, \qquad \widetilde{\theta}_b|_{\partial\Omega} = \theta_b\,, \qquad \widetilde{c}_b|_{\partial\Omega} = c_b\,.
$$

Then the functions $\boldsymbol{v}$, p, θ, c are a *weak solution* of the problem (1.1)–(1.8) if

$$
\boldsymbol{v} \in H^1(\Omega)^3\,, \quad p \in L^2_0(\Omega)\,, \quad \theta \in H^1(\Omega)\,, \quad c \in H^1(\Omega)\,, \tag{2.1}
$$

$$
\boldsymbol{v} - \widetilde{\boldsymbol{v}}_b \in \mathbf{W}\,, \quad \theta - \widetilde{\theta}_b \in \Theta\,, \quad c - \widetilde{c}_b \in \mathcal{C} \tag{2.2}
$$

and

$$
\begin{aligned}
a_1(\boldsymbol{v},\boldsymbol{w}) + \alpha_5\,b_1(\boldsymbol{v},\boldsymbol{v},\boldsymbol{w}) + \alpha_5\,b(\boldsymbol{w},p) \ &= \ \alpha_1<\mathrm{F}_1(\theta),\boldsymbol{w}> + \alpha_2<\mathrm{F}_2(c),\boldsymbol{w}> -\\
&\quad - \alpha_3\,d(\theta,\boldsymbol{w}) - \alpha_4\,d(c,\boldsymbol{w}) \qquad \forall\ \boldsymbol{w} \in \mathbf{W}\,,
\end{aligned} \tag{2.3}
$$

$$
b(\boldsymbol{v},\lambda) \ = \ 0 \qquad \forall\ \lambda \in L^2_0(\Omega)\,, \tag{2.4}
$$

$$
a_2(\theta,\eta) + \alpha_6\,b_2(\boldsymbol{v},\theta,\eta) \ = \ <\Phi_1(\theta),\eta> \qquad \forall\ \eta \in \Theta\,, \tag{2.5}
$$

$$
a_2(c,q) + \alpha_7\,b_2(\boldsymbol{v},c,q) \ = \ <\Phi_2(c),q\,\boldsymbol{v}_b> \qquad \forall\ q \in \mathcal{C}\,. \tag{2.6}
$$

Remark 2.1 If Γ^{LG} is plane, then, in (2.3), the bilinear form a_1 can be replaced by the bilinear form $\int_\Omega \nabla \boldsymbol{v} \cdot \nabla \boldsymbol{w} \, \mathrm{d}x$ and the formula for d can be simplified.

It is easy to show that any classical solution of the problem (1.1)–(1.8) is a weak solution and that, on the contrary, any sufficiently regular weak solution is a classical solution. If $\alpha_1, \dots, \alpha_7$, $\boldsymbol{f}_1(0)$, $\boldsymbol{f}_2(0)$, K_1, K_2, L_1, L_2, $\boldsymbol{v}_b$, θ_b, c_b are sufficiently small, then it can be shown that the problem (1.1)–(1.8) has at most one weak solution. Finally, using the Leray–Schauder principle and a simple scaling argument, it is possible to prove that, under the additional assumption

$$\exists\, \varepsilon \in (0,1) \quad \forall\, \boldsymbol{v} \in \mathbf{V} \quad \exists\, \widetilde{\boldsymbol{v}}_b \in H^1(\Omega)^3 : \quad \operatorname{div} \widetilde{\boldsymbol{v}}_b = 0 \,,$$
$$\widetilde{\boldsymbol{v}}_b|_{\Gamma^W \cup \Gamma^{LS}} = \boldsymbol{v}_b \,, \quad \widetilde{\boldsymbol{v}}_b \cdot \boldsymbol{n}|_{\Gamma^{LG}} = 0 \,, \qquad b_1(\boldsymbol{v}, \boldsymbol{v}, \widetilde{\boldsymbol{v}}_b) \le \frac{\varepsilon}{\alpha_5}\, a_1(\boldsymbol{v}, \boldsymbol{v}) \,,$$

there exists at least one weak solution of the problem (1.1)–(1.8).

3 Finite Element Discretization

For defining a finite element discretization of the problem (1.1)–(1.8), we introduce a tetrahedral triangulation $\mathcal{T}_h = \{T\}$ of the domain Ω (cf. [2], p. 61) and denote by Ω_h the interior of the union of the elements T of $\mathcal{T}_h$. All the domains Ω_h are contained in some bounded domain $\widetilde{\Omega}$ with a Lipschitz–continuous boundary. The sets Γ^W, Γ^{LG}, Γ^{LS} are approximated by relatively open sets Γ_h^W, Γ_h^{LG}, $\Gamma_h^{LS} \subset \partial\Omega_h$, respectively, consisting of whole faces. We assume that the triangulations possess the usual properties and form a regular family. Generally, $\Omega_h \neq \Omega$, which complicates investigations of the properties of the discrete problems. Moreover, since the normal vector to the boundary of Ω_h then differs from the normal vector $\boldsymbol{n}$, it is difficult to formulate a suitable discrete version of the condition $\boldsymbol{v} \cdot \boldsymbol{n} = 0$ on Γ^{LG}.

For proving optimal convergence results, some additional assumptions to those ones from Section 1 are necessary. We suppose that $\boldsymbol{m} \in W^{2,\infty}(\mathbb{R}^3)^3$ and that the first derivatives of the functions $\boldsymbol{f}_1$, $\boldsymbol{f}_2$, φ_1, φ_2 are Lipschitz–continuous. Further, we assume that the sets int $\overline{\Gamma^W \cup \Gamma^{LS}}$ and int $\overline{\Gamma^W \cup \Gamma^{LG}}$ are of class $C^{0,1*}$ (cf. below) and that each of the sets Γ^W, Γ^{LG} and Γ^{LS} consists of a finite number of C^2 surfaces of class $C^{0,1*}$ having piecewise C^2 boundaries. The triangulations are assumed to take into account the boundaries of the C^2 parts of $\partial\Omega$ and the points where a C^2 regularity of these boundaries is not available. The $C^{0,1*}$ property is introduced in the following definition.

Definition 3.1 A relatively open set $\Gamma \subset \partial\Omega$ is of class $C^{0,1*}$ if there exists a finite number of local Cartesian coordinate systems providing a description of $\partial\Omega$ (cf. [5], p. 14) such that, in each of these coordinate systems, the projection of the respective part of Γ into the (x_1, x_2)–plane is a set with a Lipschitz–continuous boundary.

We assume that we are given piecewise polynomial finite element spaces $\widehat{\mathbf{W}}_h$, M_h, $\widehat{\Theta}_h$ and $\widehat{\mathcal{C}}_h$ satisfying

$$\widehat{\mathbf{W}}_h \subset H^1(\Omega_h)^3 \,, \quad \mathrm{M}_h \subset L_0^2(\Omega_h) \,, \quad \widehat{\Theta}_h \subset H^1(\Omega_h) \,, \quad \widehat{\mathcal{C}}_h \subset H^1(\Omega_h)$$

and approximating the spaces $\widehat{\mathbf{W}}$, $L^2_0(\Omega)$, $H^1(\Omega)$ and $H^1(\Omega)$, respectively, and we set

$$\mathbf{W}_h = \{\boldsymbol{v} \in \widehat{\mathbf{W}}_h \mid \boldsymbol{v} = \mathbf{0} \ \text{ on } \ \Gamma_h^W \cup \Gamma_h^{LS}\}\,,$$
$$\Theta_h = \{\theta \in \widehat{\Theta}_h \mid \theta = 0 \ \text{ on } \ \Gamma_h^W \cup \Gamma_h^{LS}\}\,, \qquad \mathcal{C}_h = \{c \in \widehat{\mathcal{C}}_h \mid c = 0 \ \text{ on } \ \Gamma_h^W \cup \Gamma_h^{LG}\}\,.$$

We assume that the spaces $\mathbf{W}_h$, M_h, Θ_h and $\mathcal{C}_h$ possess the following approximation properties.

A1: There exist an integer $l \in \{2,3\}$ and an operator $r_h \in \mathcal{L}(\mathbf{W} \cap H^l(\Omega)^3, \mathbf{W}_h)$ such that

$$\|\boldsymbol{v} - r_h\,\boldsymbol{v}\|_{1,\Omega_h} \le C\,h^{\frac{l}{2}}\,\|\boldsymbol{v}\|_{l,\widetilde{\Omega}} \qquad \forall\ \boldsymbol{v} \in H^l(\widetilde{\Omega})^3\,,\ \boldsymbol{v}|_\Omega \in \mathbf{W}\,.$$

The property $\boldsymbol{v}\cdot\boldsymbol{n} = 0$ on Γ^{LG} is approximated by $\mathbf{W}_h$ in such a way that either (if $l = 2$)

$$\|\boldsymbol{v}_h \cdot \boldsymbol{n}_h\|_{0,\frac{4}{3},\Gamma_h^{LG}} \le C\,h\,\|\boldsymbol{v}_h\|_{1,\Omega_h} \qquad \forall\ \boldsymbol{v}_h \in \mathbf{W}_h\,,$$

where $\boldsymbol{n}_h$ is the unit outward normal vector to $\partial\Omega_h$, or (if $l = 3$)

$$\|\boldsymbol{v}_h \cdot \bar{\boldsymbol{n}}_h\|_{0,1,\Gamma_h^{LG}} \le C\,h^{\frac{3}{2}}\,\|\boldsymbol{v}_h\|_{1,\Omega_h} \qquad \forall\ \boldsymbol{v}_h \in \mathbf{W}_h\,,$$

where $\bar{\boldsymbol{n}}_h \in L^2(\partial\Omega_h)^3$ is the piecewise linear interpolate of the unit outward normal vector $\boldsymbol{n}$ to $\partial\Omega$. In addition, we assume that any $\boldsymbol{v}_h \in \mathbf{W}_h$ satisfies $\boldsymbol{v}_h \cdot \boldsymbol{n}_h^* = 0$ in any vertex of $\mathcal{T}_h$ lying in Γ_h^{LG}, where $\boldsymbol{n}_h^*$ is a function defined in the vertices of $\mathcal{T}_h$ and satisfying for some fixed $\alpha \in (0, 1>$

$$|\boldsymbol{n}_h^*(x) - \boldsymbol{n}(x)| \le C\,h_T^{1+\alpha} \quad \text{in any vertex } x \in \Gamma_h^{LG},$$

with $T \in \mathcal{T}_h$ being any element containing the vertex x.

A2: There exists an operator $s_h \in \mathcal{L}(L^2_0(\Omega) \cap H^{l-1}(\Omega), \mathrm{M}_h)$ such that

$$\|p - s_h\,p\|_{0,\Omega_h} \le C\,h^{\frac{l}{2}}\,\|p\|_{l-1,\widetilde{\Omega}} \qquad \forall\ p \in H^{l-1}(\widetilde{\Omega})\,,\ p|_\Omega \in L^2_0(\Omega)\,.$$

A3: There exists an operator $t_h \in \mathcal{L}(\Theta \cap H^l(\Omega), \Theta_h)$ such that

$$\|\theta - t_h\,\theta\|_{1,\Omega_h} \le C\,h^{\frac{l}{2}}\,\|\theta\|_{l,\widetilde{\Omega}} \qquad \forall\ \theta \in H^l(\widetilde{\Omega})\,,\ \theta|_\Omega \in \Theta\,.$$

A4: There exists an operator $\tau_h \in \mathcal{L}(\mathcal{C} \cap H^l(\Omega), \mathcal{C}_h)$ such that

$$\|c - \tau_h\,c\|_{1,\Omega_h} \le C\,h^{\frac{l}{2}}\,\|c\|_{l,\widetilde{\Omega}} \qquad \forall\ c \in H^l(\widetilde{\Omega})\,,\ c|_\Omega \in \mathcal{C}\,.$$

A5: There exists a constant $\beta^* > 0$ independent of h such that

$$\sup_{\boldsymbol{v}_h \in \mathbf{W}_h, \boldsymbol{v}_h \ne \mathbf{0}} \frac{\int_{\Omega_h} \lambda_h \operatorname{div} \boldsymbol{v}_h \,\mathrm{d}x}{\|\boldsymbol{v}_h\|_{1,\Omega_h}} \ge \beta\,\|\lambda_h\|_{0,\Omega_h} \qquad \forall\ \lambda_h \in \mathrm{M}_h\,.$$

A discretization of the problem (1.1)–(1.8) have the same structure as its weak formulation and is given in the following definition. The used mappings are defined below.

Definition 3.2 The functions $\boldsymbol{v}_h$, p_h, θ_h, c_h are a *discrete solution* of the problem (1.1)–(1.8) if

$$\boldsymbol{v}_h - \widetilde{\boldsymbol{v}}_{bh} \in \mathbf{W}_h \,, \quad \theta_h - \widetilde{\theta}_{bh} \in \Theta_h \,, \quad c_h - \widetilde{c}_{bh} \in \mathcal{C}_h \tag{3.1}$$

and

$$\begin{aligned} &a_{1h}(\boldsymbol{v}_h, \boldsymbol{w}_h) + \alpha_5\, b_{1h}(\boldsymbol{v}_h, \boldsymbol{v}_h, \boldsymbol{w}_h) + \alpha_5\, b_h(\boldsymbol{w}_h, p_h) = \alpha_1 <\mathrm{F}_{1h}(\theta_h), \boldsymbol{w}_h> + \\ &\quad + \alpha_2 <\mathrm{F}_{2h}(c_h), \boldsymbol{w}_h> - \alpha_3\, d_h(\theta_h, \boldsymbol{w}_h) - \alpha_4\, d_h(c_h, \boldsymbol{w}_h) \qquad \forall\, \boldsymbol{w}_h \in \mathbf{W}_h \,, \end{aligned} \tag{3.2}$$

$$b_h(\boldsymbol{v}_h, \lambda_h) = 0 \qquad \forall\, \lambda_h \in \mathrm{M}_h \,, \tag{3.3}$$

$$a_{2h}(\theta_h, \eta_h) + \alpha_6\, b_{2h}(\boldsymbol{v}_h, \theta_h, \eta_h) = <\Phi_{1h}(\theta_h), \eta_h> \qquad \forall\, \eta_h \in \Theta_h \,, \tag{3.4}$$

$$a_{2h}(c_h, q_h) + \alpha_7\, b_{2h}(\boldsymbol{v}_h, c_h, q_h) = <\Phi_{2h}(c_h), q_h> \qquad \forall\, q_h \in \mathcal{C}_h \,. \tag{3.5}$$

The Dirichlet boundary conditions are now approximated by traces of some suitable functions $\widetilde{\boldsymbol{v}}_{bh} \in \widehat{\mathbf{W}}_h$, $\widetilde{\theta}_{bh} \in \widehat{\Theta}_h$ and $\widetilde{c}_{bh} \in \widehat{\mathcal{C}}_h$. The mappings a_{1h}, a_{2h}, b_{1h}, b_{2h}, F_{1h} and F_{2h} are defined similarly as a_1, a_2, etc. in Section 2 – only the integration is done over the domain Ω_h instead of Ω. In the same way, we can define a discrete analogue d_h^* of d:

$$d_h^*(\zeta_h, \boldsymbol{w}_h) = \int_{\Omega_h} \nabla\zeta_h \cdot [\, \boldsymbol{w}_h \operatorname{div} \boldsymbol{m} - \boldsymbol{m} \operatorname{div} \boldsymbol{w}_h + (\nabla \boldsymbol{w}_h)\, \boldsymbol{m} - (\nabla \boldsymbol{m})\, \boldsymbol{w}_h]\, \mathrm{d}x \,,$$

where ζ_h stands for θ_h or c_h. However, it would generally be too expensive to compute $d_h^*(\zeta_h, \boldsymbol{w}_h)$ exactly and therefore we use some easier computable mapping $d_h : C(\overline{\Omega}_h) \times \mathbf{W}_h \to \mathbb{R}$ satisfying

$$|d_h^*(\zeta_h, \boldsymbol{w}_h) - d_h(\zeta_h, \boldsymbol{w}_h)| \leq C\, h^{\frac{l}{2}}\, \|\zeta_h\|_{1,\Omega_h}\, \|\boldsymbol{w}_h\|_{1,\Omega_h} \qquad \forall\, \zeta_h \in \widehat{\Theta}_h \cup \widehat{\mathcal{C}}_h \,,\ \boldsymbol{w}_h \in \mathbf{W}_h \,,$$

where the integer l is the same as in the assumptions A1–A4. The two basic ways to define the mapping d_h are to evaluate d_h^* by means of a numerical integration or to replace the function $\boldsymbol{m}$ in the definition of d_h^* by a polynomial interpolate of $\boldsymbol{m}$. The second possibility is more advantageous since d_h then (similarly as d_h^*) vanishes for $\boldsymbol{w}_h \in \mathbf{W}_h \cap H_0^1(\Omega_h)^3$.

The functionals $\Phi_{1h}(\theta)$ and $\Phi_{2h}(c)$ are defined by

$$<\Phi_{1h}(\theta), \eta> = -\int_{\Gamma_h^{LG}} \eta\, \varphi_1(\theta)\, \mathrm{d}\sigma \,, \qquad <\Phi_{2h}(c), q> = -\int_{\Gamma_h^{LS}} q\, (\widetilde{\boldsymbol{v}}_{bh} \cdot \widetilde{\boldsymbol{n}}_h)\, \varphi_2(c)\, \mathrm{d}\sigma \,,$$

where $\widetilde{\boldsymbol{n}}_h \in L^2(\partial\Omega_h)^3$ is an approximation of the normal vector $\boldsymbol{n}$ to $\partial\Omega$. If the assumptions A1–A4 hold with $l = 3$, we assume that $\widetilde{\boldsymbol{n}}_h$ is the piecewise linear interpolate of $\boldsymbol{n}$. If $l = 2$, it is sufficient to use the unit outward normal vector to $\partial\Omega_h$.

The following theorem shows that the above assumptions guarantee optimal convargence properties of the discrete solutions.

Theorem 3.1 *Let the above assumptions be satisfied and let $\boldsymbol{m} \in W^{l,\infty}(\widetilde{\Omega})^3$, where l is the constant from the assumptions A1–A4. Let $\mathrm{U} = (\boldsymbol{v}, p, \theta, c)$ be a nonsingular weak solution of the problem (1.1)–(1.8). Let $\mathrm{P} \in \mathcal{L}(H^1(\Omega), H^1(\widetilde{\Omega}))$ be an extension operator defined by means of the Nikolskij method (cf. [5], p. 75, Theorem 3.9) and let the functions from (2.2) and (3.1) satisfy*

$$\lim_{h\to 0} \Big\{ \|\mathrm{P}\,\widetilde{\boldsymbol{v}}_b - \widetilde{\boldsymbol{v}}_{bh}\|_{1,\Omega_h} + \|\mathrm{P}\,\widetilde{\theta}_b - \widetilde{\theta}_{bh}\|_{1,\Omega_h} + \|\mathrm{P}\,\widetilde{c}_b - \widetilde{c}_{bh}\|_{1,\Omega_h} \Big\} = 0\,.$$

Then there exist constants $h_0 > 0$ and $R > 0$ such that, for $h \in (0, h_0)$, the discrete problem (3.1)–(3.5) has a solution $\mathrm{U}_h = (\boldsymbol{v}_h, p_h, \theta_h, c_h)$ which is unique in a ball with a diameter R and the centre in an extension of U. *This unique solution is nonsingular and satisfies*

$$\lim_{h\to 0} \Big\{ \|\mathrm{P}\,\boldsymbol{v} - \boldsymbol{v}_h\|_{1,\Omega_h} + \|p - p_h\|_{0,\Omega_h} + \|\mathrm{P}\,\theta - \theta_h\|_{1,\Omega_h} + \|\mathrm{P}\,c - c_h\|_{1,\Omega_h} \Big\} = 0\,,$$

where p is considered as extended by zero outside Ω. If, in addition, $\boldsymbol{v}$, $\widetilde{\boldsymbol{v}}_b \in H^l(\Omega)^3$, $p \in H^{l-1}(\Omega)$, θ, $\widetilde{\theta}_b$, c, $\widetilde{c}_b \in H^l(\Omega)$, where l is the constant from the assumptions A1–A4, Γ^{LG} and Γ^{LS} are piecewise C^l, and

$$\|\overline{\mathrm{P}}\,\widetilde{\boldsymbol{v}}_b - \widetilde{\boldsymbol{v}}_{bh}\|_{1,\Omega_h} + \|\overline{\mathrm{P}}\,\widetilde{\theta}_b - \widetilde{\theta}_{bh}\|_{1,\Omega_h} + \|\overline{\mathrm{P}}\,\widetilde{c}_b - \widetilde{c}_{bh}\|_{1,\Omega_h} \le C\, h^{\frac{l}{2}}\,,$$

where $\overline{\mathrm{P}} \in \mathcal{L}(H^l(\Omega), H^l(\widetilde{\Omega}))$ is an arbitrary extension operator, then there exists $h_1 \in (0, h_0)$ and $C > 0$ such that, for $h \in (0, h_1)$,

$$\|\overline{\mathrm{P}}\,\boldsymbol{v} - \boldsymbol{v}_h\|_{1,\Omega_h} + \|\widetilde{\mathrm{P}}\,p - p_h\|_{0,\Omega_h} + \|\overline{\mathrm{P}}\,\theta - \theta_h\|_{1,\Omega_h} + \|\overline{\mathrm{P}}\,c - c_h\|_{1,\Omega_h} \le C\, h^{\frac{l}{2}}\,,$$

where $\widetilde{\mathrm{P}} \in \mathcal{L}(H^{l-1}(\Omega), H^{l-1}(\widetilde{\Omega}))$ is an arbitrary extension operator.

Proof. The proof is based on the abstract theory of the approximation of branches of nonsingular solutions and requieres many auxiliary results, the proofs of which are rather technical. Details can be found in [4]. □

4 Numerical Solution of the Discrete Problem

In this section we deal with the numerical solution of the discretization from Section 3 without the equation for concentration. The constants $\alpha_1, \ldots, \alpha_6$ and the functions $\boldsymbol{f}_1$ and φ_1 are defined as in Remark 1.1. The dimensionless parameters are given by

$$\begin{aligned} &Re = 1.79 \cdot 10^4\,, \quad Pr = 2.40 \cdot 10^{-2}\,, \quad Gr_\theta = 2.91 \cdot 10^8\,, \quad Ma_\theta = 8.74 \cdot 10^4\,,\\ &Bi = 0\,, \quad Rd = 1.30 \cdot 10^{-6}\,, \quad \widetilde{\theta} = 46.0\,, \quad \theta_{inf} = -7.34\,, \end{aligned}$$

which are physically realistic values. We consider a rotationally symmetrical computational domain Ω of the type used in the Czochralski method. The used triangulation of Ω comprises 51840 tetrahedra and its front view is shown in Fig. 2. The radius of

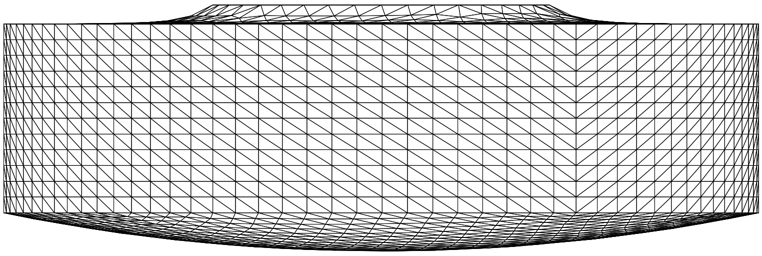

Figure 2 Front view of the triangulation.

the domain Ω is 1 and the maximum height is 0.65. The Dirichlet boundary conditions are defined by

$$\begin{aligned} \boldsymbol{v}_b &= \frac{1}{2\,\pi}\,(-x_2, x_1, 0)\,, \qquad \theta_b = \frac{-3 + 40\,(x_1^2 + x_2^2)}{74} \qquad \text{on } \Gamma^W\,,\\ \boldsymbol{v}_b &= -\frac{1}{\pi}\,(-x_2, x_1, 0)\,, \qquad \theta_b = -\frac{1}{2} \qquad \text{on } \Gamma^{LS}\,. \end{aligned}$$

The space M_h consists of piecewise constant functions and the space $\widehat{\Theta}_h$ of continuous piecewise linear functions. Then M_h and Θ_h satisfy the assumptions A2 and A3 with $l = 2$. The construction of a suitable space $\widehat{\mathbf{W}}_h$ is more difficult. First, we consider a space $\widehat{\mathbf{W}}_h^1$ consiting of continuous piecewise linear functions $\boldsymbol{v}_h$ satisfying $(\boldsymbol{v}_h \cdot \boldsymbol{n}_h^*)(x) = 0$ in any vertex $x \in \Gamma_h^{LG}$, where $\boldsymbol{n}_h^*(x)$ is a weighted average of the normal vectors to the boundary faces containing the vertex x. This is sufficient for satisfying the assumption A1 with $l = 2$, however, $\widehat{\mathbf{W}}_h^1$ is to small to satisfy the assumption A5. Therefore, we set $\widehat{\mathbf{W}}_h = \widehat{\mathbf{W}}_h^1 \oplus \widehat{\mathbf{W}}_h^2$, where $\widehat{\mathbf{W}}_h^2 \subset H_0^1(\Omega)^3$ is a space generated by piecewise cubic vector functions in the directions of normal vectors to the inner faces of the triangulation (see [3], p. 145). Due to the special definiton of $\boldsymbol{n}_h^*$, we have $\int_{\partial\Omega_h} \boldsymbol{w}_h \cdot \boldsymbol{n}_h \,\mathrm{d}\sigma = 0$ for any $\boldsymbol{w}_h \in \mathbf{W}_h$. Thus, if $\int_{\partial\Omega_h} \widetilde{\boldsymbol{v}}_{bh} \cdot \boldsymbol{n}_h \,\mathrm{d}\sigma = 0$, the discrete velocity satisfies $b_h(\boldsymbol{v}_h, 1) = 0$ and hence characteristic functions of the elements of the triangulation can be used as the test functions q_h.

To stabilize the discretization with respect to Re, we replace a_{1h} in (3.2) by

$$a_{1h}^{Re}(\boldsymbol{v}_h, \boldsymbol{w}_h) = a_{1h}(\boldsymbol{v}_h, \boldsymbol{w}_h) + (Re - 1)\, a_{1h}(\boldsymbol{v}_h^2, \boldsymbol{w}_h^2)\,, \qquad \boldsymbol{v}_h, \boldsymbol{w}_h \in \widehat{\mathbf{W}}_h\,,$$

where $\boldsymbol{v}_h^2$, $\boldsymbol{w}_h^2$ are the uniquely determined components of $\boldsymbol{v}_h$, $\boldsymbol{w}_h$ belonging to $\widehat{\mathbf{W}}_h^2$. Theorem 3.1 also remains valid for the discrete problem with this new bilinear form. As the mapping d_h we use d_h^* with $\boldsymbol{m}$ replaced by its linear interpolate.

Introducing the usual bases in the discrete spaces, the discrete problem can be equivalently written as a system of 1.83×10^5 nonlinear algebraic equations for the coefficients of the discrete solution. A linearization is done replacing the first argument in the terms $b_{1h}(\boldsymbol{v}_h, \boldsymbol{v}_h, \boldsymbol{w}_h)$ and $b_{2h}(\boldsymbol{v}_h, \theta_h, \eta_h)$ by the velocity from the previous step. The equation for the temperature is then independent of the Navier–Stokes equations and can be solved using the GMRES method. The computed temperature is substituted in the Navier–Stokes equations and new velocity and pressure approximations

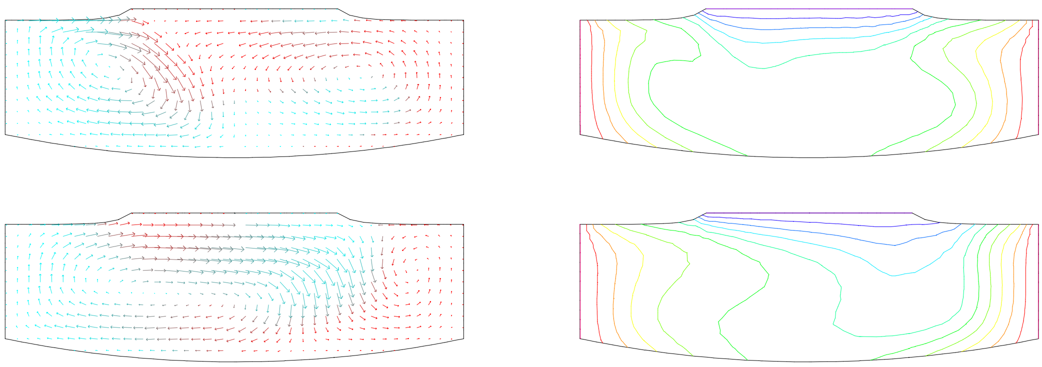

Figure 3 Velocity vectors and temperature isolines in two vertical cross–sections.

are computed by means of the augmented Lagrangian method. The computation was terminated when relative defects were smaller than 10^{-6}.

The results of the computation are presented in Fig. 3, where velocity vectors and temperature isolines in two different vertical cross–section planes are shown. The Figures 2 and 3 were created using the visualization program GRAPE developed at the universities of Bonn and Freiburg. Both the velocity and the temperature distributions are asymmetric, which is in correspondence with experiments (cf. e.g. [7]) and indicates the necessity to use nonstationary models.

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