A flow driven by free convection and a magnetic field - numerical modeling and optimization

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Abstract. To optimize processes in chemical engineering and material sciences nowadays is an important issue. Based on mathematical models the optimization goal for example consists in maximizing the output of a process, or in optimizing the quality of a produced material. This work focusses on the optimization of thermally coupled flows as they occur in growth processes from a melt influenced by thermal and magnetic fields.

There are several stages of modeling and we consider first the influence of a magnetic field via the Lorentz force source term in the impuls balance. Here we discuss two kinds of magentic fields, the RMF (rotating magnetic field) and the TMF (travelling magnetic field). The parameters of the Lorentz force terms serve as control variables with respect to the optimization. This paper is sequel of the work of [1].

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THE MATHEMATICAL MODEL

In many crystal growth processes the flow and the temperature gradients in the melt have a considerable impact on the quality of the crystal. The stationary flow is governd by the Boussinesq approximation for a velocity-pressure-temperature field $(\mathbf{U}, P, T)$ in the flow domain Ω;

$$\rho(\vec{U}\cdot\nabla)\vec{U} = -\nabla P + \eta\Delta\vec{U} + \rho\vec{g}\beta(T-T_0) + \vec{j}\times\vec{B} \tag{1}$$

$$-\nabla\cdot\vec{U} = 0 \tag{2}$$

$$\rho c_p \vec{U}\cdot\nabla T - \lambda\Delta T = 0\ , \tag{3}$$

and a simplification including time averaging over a period gives for the z- and the φ-direction of the Lorentz force $\vec{f}^L = \vec{j}\times\vec{B}$

$$f_z^L = \frac{\sigma\omega_T B_T^2 k}{8} r^2 \qquad f_\varphi^L = \frac{\sigma\omega_R B_R^2}{2\rho} r f_c\ . \tag{4}$$

The parameters $\sigma_{T,R}$, $\omega_{T,R}$, $B_{T,R}$, k and f_c characterize the TMF and RMF.

The expressions (4) for $\vec{f}^L$ could be directly inserted into the momentum equation with the result

$$(\vec{U}\cdot\nabla)\vec{U} = -\frac{1}{\rho}\nabla P + \nu\Delta\vec{U} + \frac{\sigma\omega_R B_R^2}{2\rho} r f_c \vec{e}_\varphi + (g_z\beta(T-T_0) + \frac{\sigma\omega B_0^2 k}{8\rho} r^2)\vec{e}_z\ . \tag{5}$$

Because of the special configuration of our problem (see also Fig. 1) we can assume a cylindrical problem region and a homogeneity in the φ-direction with

$$\frac{\partial\Psi}{\partial\varphi} = 0$$

for all quatities $\Psi = \vec{U}, P, T$.

To have an idea of the typical problem parameters Taylor number Ta and dimensionless Lorentz force density F we do a non-dimensionalisation with the scales R (a crucible radius) for distance, R^2/ν for time, $\rho\nu^2/R^2$ for pressure and ν/R for velocity. For the dimensionless velocity $(u, v, w) = (u_r, u_z, u_\varphi)$ pressure p and temperature θ fields we get the

Navier-Stokes equation in cylindrical coordinates (r,φ,z) as follows.

$$u\frac{\partial u}{\partial r}+v\frac{\partial u}{\partial z}=-\frac{\partial p}{\partial r}+\Delta u-\frac{u}{r^2}+\frac{w^2}{r} \tag{6}$$

$$u\frac{\partial w}{\partial r}+v\frac{\partial w}{\partial z}=\Delta w-\frac{uw}{r}-\frac{w}{r^2}+Ta_R r f_c \tag{7}$$

$$u\frac{\partial v}{\partial r}+v\frac{\partial v}{\partial z}=-\frac{\partial p}{\partial z}\Delta v+Gr\,\theta+\frac{1}{2}F_T r^2 , \tag{8}$$

with the Taylor number, the dimensionless Lorentz force density and the Grashof number

$$Ta_R=\frac{\sigma\omega_R B_R^2 R^4}{2\rho v^2} , \quad F_T=\frac{\sigma\omega_T B_T^2 k R^5}{4\rho v^2} , \quad Gr=\frac{g_z\beta(T_b-T_t)R^3}{v^2} . \tag{9}$$

For the dimensionless temperature $\theta=\frac{T-T_t}{T_b-T_t}$ with the top temperature $T_t$less than the bottom temperature T_b we get the convective heat conduction equation

$$u\frac{\partial\theta}{\partial r}+v\frac{\partial\theta}{\partial z}=\frac{1}{Pr}\Delta\theta . \tag{10}$$

Pr is here the Prandtl number. The continuity equation reads as

$$\frac{1}{r}\frac{\partial ru}{\partial r}+\frac{\partial v}{\partial z}=0 . \tag{11}$$

We summarize the whole non-dimensional model equation system in vectorial writing style to

$$(\vec{u}\cdot\nabla)\vec{u}-\Delta\vec{u}+\nabla p-Ta_R r f_c\vec{e}_\varphi--Gr\theta\vec{e}_z-\frac{1}{2}F_T r^2\vec{e}_z \quad = \quad 0 \tag{12}$$

$$\nabla\cdot\vec{u}=0 \tag{13}$$

$$(\vec{u}\cdot\nabla)\theta-\frac{1}{Pr}\Delta\theta \quad = \quad 0 . \tag{14}$$

Fig. 1 shows the experimental configuration of the group of G. Gerbeth [2], who inspired us to investigate the configuration theoretically. The boundary conditions for the velocity are no slip conditions at solid walls and

$$\vec{u}\cdot\vec{n}=0 , \quad \frac{\partial\vec{u}\cdot\vec{t}}{\partial\vec{t}}=0 ,$$

for the normal and tangential velocity component at the free surface of the melt. For the temperatures we have Dirichlet boundary conditions for the bottom of the crucible and the interface between the melt and the solid crystal (melting temperature). At the side walls of the crucible and the free surface we use adiabatic boundary conditions for the temperature.

The goal of the parameter studies and a possible optimization problem is achieved by minimizing a cost functional of the form

$$J(\theta,Ta,F)=\frac{1}{2}\int_{\Omega_0}|\nabla\theta|^2 d\Omega_0 \quad \text{s.t.} \quad (12),(13),(14) , \tag{15}$$

where Ω_0 means a small subregion of Ω near the triple point of the melt, the solid crystal and the free surface.

NUMERICAL MODEL

The numerical solution procedure for the system (12),(13),(14) consists in

1) spatial discretization: **FEM-method**,
2) nonlinear system solver: **conjugate gradient/Newton method**.

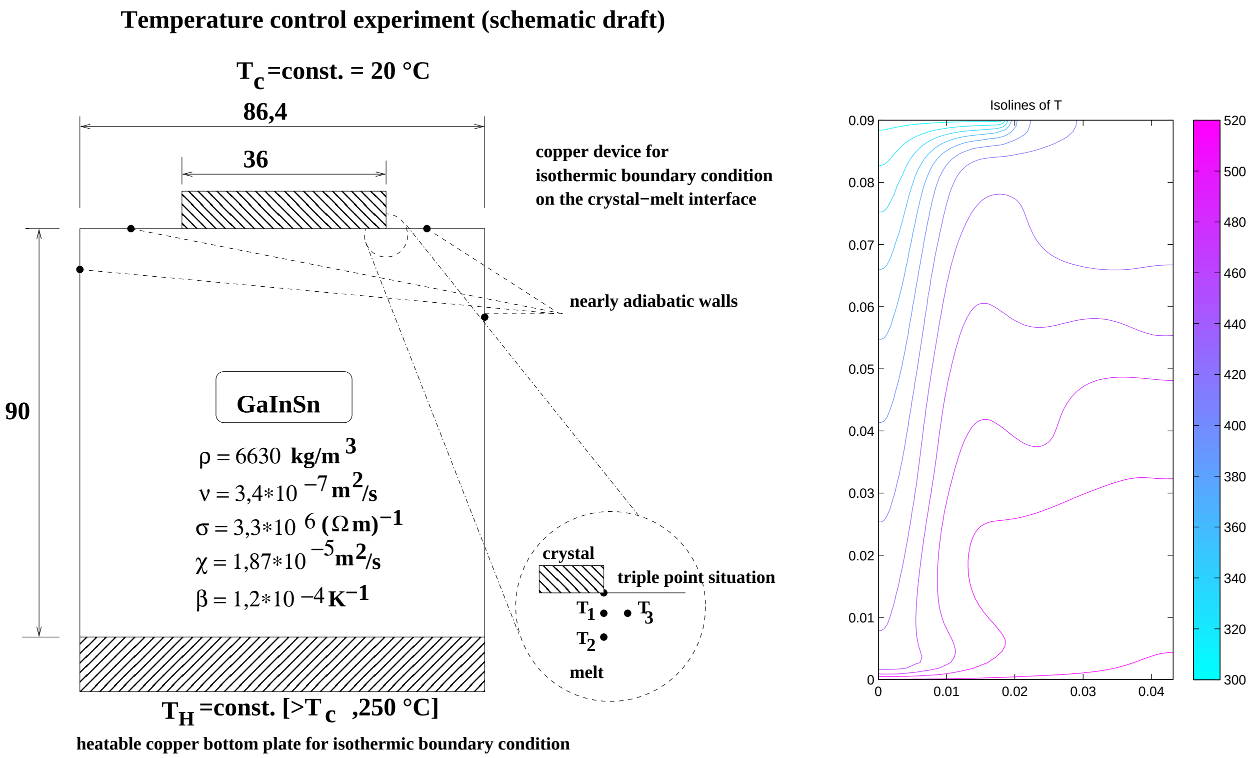

FIGURE 1. Problem configuration (left) and a typical temperature field

The procedure is realized for the 2.5D problem using tools of the package *Comsol multiphysics*. On the other hand there are also computations with the FEM-package *Entwife* of A. Cliffe [3], which confirm the results of the computations with *Comsol multiphysics*.

The study of the functional (15) and its minimization is still under consideration. In a first stage we evaluate the gradient of J by finite differences. The use of the adjoint calculus following [4] with the aim of a Karush-Kuhn-Tucker system to get critical points is prepared for a generalised model of the magnetic field using the Maxwell equations to describe the magnetic field caused by a given current through a conductor.

RESULTS

The parameter studies of the influence of prescribed RMF and TMF magnetic fields (Ta and/or F) are done with the fixed Grashof number 10^6 for the crystal material **GaInSn**. There were done variations of the travelling magnetic field by F_T from 0 up to 4×10^5 and variations of the rotating magnetic field by Ta_R from 0 up to 8×10^3. Fig. 2 shows typical fields of the velocity (u,v) (left) and isolines of w in a (r,z)-plane.

All parameter variations of F_T and Ta_R show an increasing of the temperature gradients near the triple point (Ω_0). In the tables the gradients ($T_z = (T_1 - T_2)/\Delta z$, $T_r = (T_3 - T_1)/\Delta_r$, $\Delta_z = \Delta_r = 1\,mm$) and the tangens of the south east angle are given. The gradients increase monotonously with F_T and Ta_R. Thus the idea or hope to reduce the temperature gradient near the triple point does not complied. In other words for controling and reducing the temperature gradient near the triple point simple TMF or RMF magnetic fields are not suitable.

It is important to note, that the used temperature boundary conditions on the crystal-melt interface and the free surface are only a coarse approximation and do not describe the real physical situation. Thus with more realistic temperature conditions it is worthwhile to do some further investigations of the influence of TMF and RMF magnetic

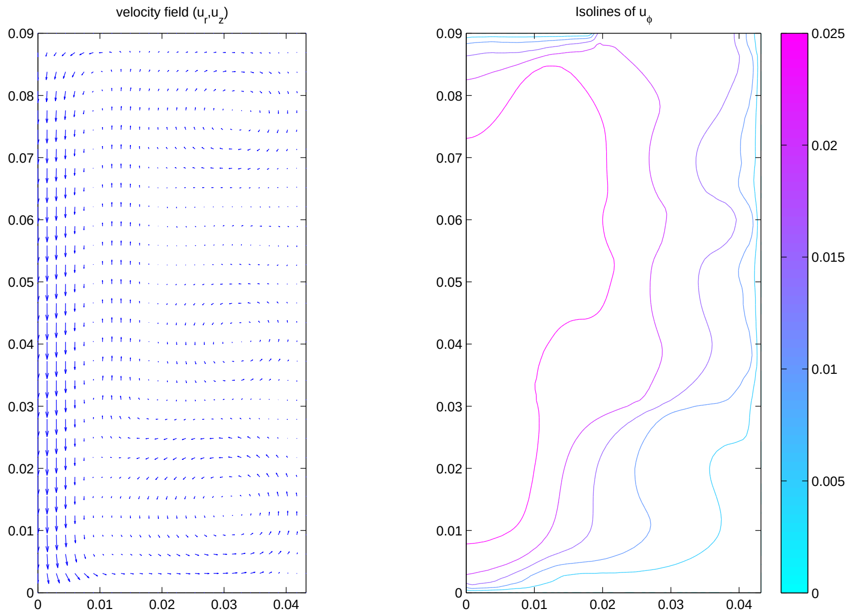

FIGURE 2. Velocity fields

fields to temperature gradient near the triple point.

F_T	norm of ∇T in [K/cm]	T_z/T_r	Ta_R	norm of ∇T in [K/cm]	T_z/T_r
0.0	940.13	-0.72818	0.0	940.13	-0.72818
10^3	940.85	-0.72811	10^3	940.99	-0.72815
10^4	947.79	-0.72814	4×10^3	952.37	-0.72895
4×10^5	1146.6	-0.72813	8×10^3	968.90	-0.73044

CONCLUSION

There must be further investigations using magnetic fields with more degrees of freedom than the simple ones of RMF- and TMF magnetic fields and more realistic temperature boundary conditions. This will be done using the coupled system of Navier-Stokes equation, convective heat conduction equation and the Maxwell equation for the magnetic flux density $\vec{B}$ which determines the Lorentz force $\vec{f}^L$.

As a control should be used the current density which is responsible for the field of the magnetic flux density. For the optimization we consider and develope now the appropriate adjoint system to evaluate the necessary optimality condition for a suitable minimization functional.

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