Crystal melt modeling and simulation with magnetic fields

Sara Heft and Günter Bärwolff

Technische Universität Berlin, Institut für Mathematik

Zusammenfassung. An aspect of recent developments in crystal growth technologies is the control of electric conductive fluids by magentic fields.
Recently it was shown by [**?**] and [**?**] that boundary control of crystal melts was not very successful.
In this paper we consider a coupled model constisting of the mass, momentum and energy balance for the melt and a global induction equation. This extensive modeling is very good base for the crystal melt control by certain magnetic fields.
We develope and dicuss the mathematical model and the numerical solution method and demonstrate some simulation results for the twodimensional and threedimensional case.
Finally on this base an outlock for a possible benefit of the considered mathematical model and its numerical solution for a flow/melt control is given.

Keywords: Navier-Stokes equation, incompressible flow, optimization, flow control
PACS: 45.70.Vn, 47.10.ad, 47.11.-j, 47.11.Df, 47.85.L-

THE DESCRIPTION OF THE METHOD

Firstly we concentrate ourself on the different model stages. The Fig. **??** shows the gemoetrical situation.

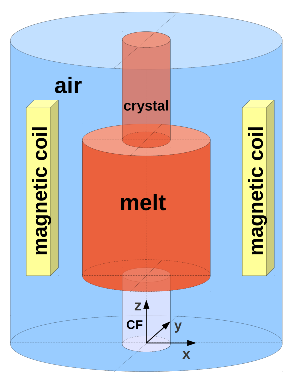

Abbildung 1. Cylindrical model region

For the mass, momentum and energy balance we have the equation system

$$\nabla \cdot \mathbf{u} = 0 \,, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \nu \Delta \mathbf{u} - \frac{1}{\rho_0} \nabla p + (1 - \beta(T - T_0))\mathbf{g} + \frac{\alpha}{\rho_0 \mu}((\nabla \times \mathbf{B}) \times \mathbf{B} \tag{2}$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = D_T \Delta T \,, \tag{3}$$

$$\frac{\partial \mathbf{B}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{B} - (\mathbf{B} \cdot \nabla)\mathbf{u} = \frac{1}{\mu \sigma} \Delta \mathbf{B} \tag{4}$$

of the continuity equation, the Boussinesq equation, the heat conduction equation and the induction equation. $\mathbf{u}$ is the velocity field, p is the pressure field and T is temperature field which live all in the crucible/melt region Ω_c.

$\mathbf{B}$ is the magnetic flux density field which lives in the whole cylindrical model region Ω_g.
We differ the model stages

(m1) axi symmetric flow in the little cylinder of the crystal melt (equations (**??**), (**??**), (**??**) in the crucible Ω_c, 2d, $\alpha = 0$),

(m2) axi symmetric flow in the crucible coupled with the induced magnetic field (equations (**??**), (**??**), (**??**) in the crucible Ω_c, equation (**??**) in Ω_g, 2d, $\alpha = 1$),

(m3) flow in the crucible coupled with the induced magnetic field (equations (**??**), (**??**), (**??**) in the crucible Ω_c, equation (**??**) in Ω_g, 3d, $\alpha = 1$) .

Simple cylinder model (m1, 2d)

For the introduction into the general problem we consider a little cylinder for the region of the crystal melt as a laminar and axi symmetric flow. Because of the homogenity assumption in the circumferential direction we can use a twodimensional model. Initial and boundary conditions for the velocity (no slip on walls and at the interface melt-solid crystal, free surface conditions at the free surface) and the temperature (hot bottom temperature linearly falling down up to the melting temperature at the interface melt-solid crystal) are taken following [**?**]. The numerical solution of the initial boundary value problem was done with the program system OpenFoam. Therefore we have the create a small wedge (s. Fig. **??**).

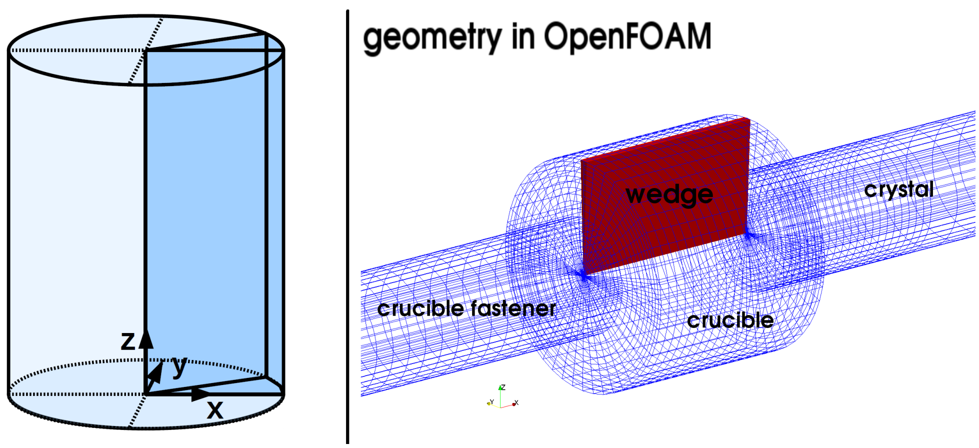

Abbildung 2. wedge geometry to describe an axi symmetric problem

The spatial discretization of the equations is done with Finite Volumes and the time discretization for the Boussinesq equation in realized by the PISO method. This is elaborated for example in [**?**] and in the OpenFoam programmers guide.

Extended cylinder model (m2, 2d)

We remark that the FV grid of the cylinder Ω_c is a subset of the FV grid of the whole cylindrical model region Ω_g. As a source for the magnetic field we prescribe the magnetic flux density on coils in Ω_g. On the outer boundary of Ω_g we use homogeneous Dirichlet data for $\mathbf{B}$. This means in OpenFoam the use of *BBoxes* which are outlined in Fig. **??**.

It could be shown that the influence of the term $(\mathbf{u}\cdot\nabla)\mathbf{B} - (\mathbf{B}\cdot\nabla)\mathbf{u}$ on the the magnetic field, i.e. the influence of the flow field on the magnetic field is negligible. Thus the coupling of the mathematical model of the flow in the crucible Ω_c wth the magnetic field is realized in two steps:

1. the computation of the magnetic flux density in Ω_g by the solution of the equation (**??**),
2. make use of the values of $\mathbf{B}$ on $\partial\Omega_c$ as Dirichlet boundary conditions for the solution of the equation system (**??**)-(**??**) in Ω_c.

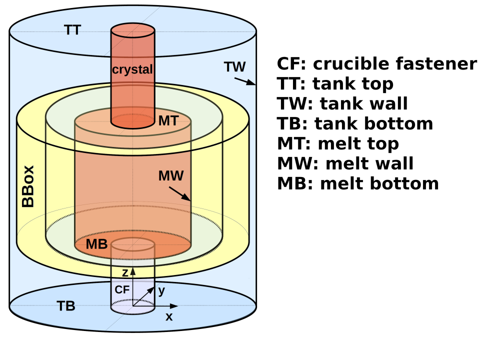

Abbildung 3. Boundary notations of the extended model

Extended cylinder model (m3, 3d)

The extension to the 3d model was straightforward. It was only necessary to extend the 2d grid of the wedge in the circumferential direction. The annular coil was realized by a few *BBoxes*. This is shown in Fig. **??**.

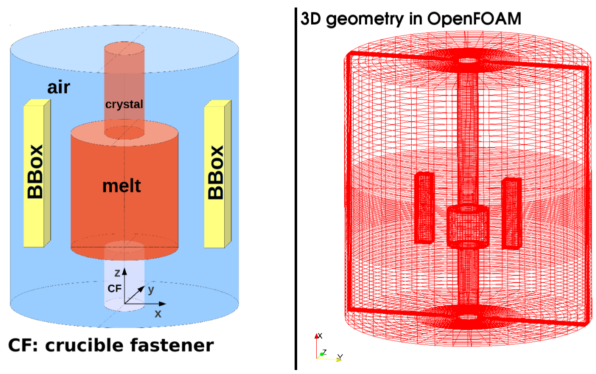

Abbildung 4. Threedimensional geometry of Ω_g (m3, 3d)

RESULTS OF NUMERICAL EXPERIMENTS

The model (m1) was used to validate the mathematical and numerical model by the solution of a benchmark of the Hartmann flow. Based on the successful validation some parameter studies with the extended 2d model (m2) are done. The prescribed magnetic flux density (source of the magnetic field) were varied from 0 *Tesla* to 2 *Tesla*. The increase of the magnitude of the magnetic flux density in the sources led to an increase of the fluid velocity and equalization of the temperature field. Fig. **??** shows the numerical experiments with different magnitudes of the magnetic field at the sources. For the magnetic field the choice of the thermal boundary condition i.e. heating boundary condition on the coat of the crucible (cases 1, 2, 4 and 6), or isolated coat of the crucible (cases 3, 5 and 7) had no consequence.
Figs. **??** and **??** show the velocity and temperature field in the crucible for the cases 0 *Tesla* and 1 *Tesla*.
A detailed documentation of the parameter test is given in [**?**].

SUMMARY

With the formulated mathematical model and the implementation of the numerics an efficient tool for description and the design of facilities for the manufacture of monocrystals was developed.
This could be the base for further investigations including the control of the melt flow and melt temperature with the aim of tracking especially desired states which guarantee a good quality of the monocrystals.

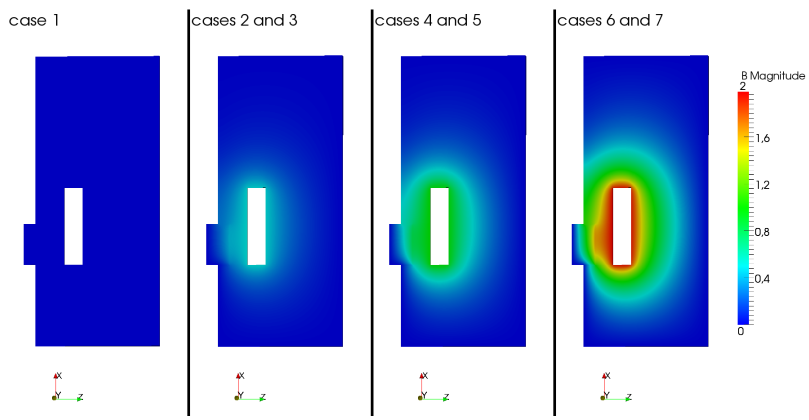

Abbildung 5. Comparison of the influence of the magnetic field for different initializations of the *BBoxes* for 0, 0.5, 1, 2 *Tesla*

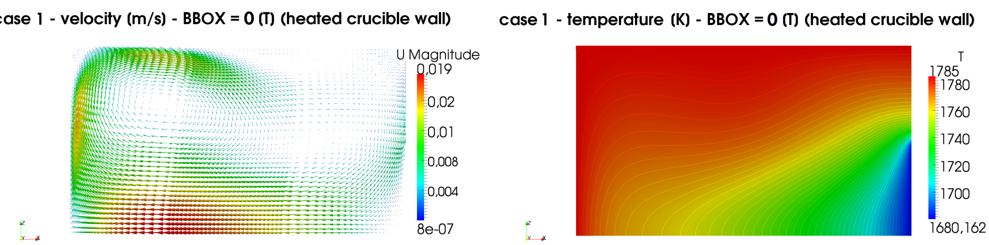

Abbildung 6. Results of numerical simulations with a heated boundary of the crucible and an initialization of the *BBoxes* with 0 *Tesla* (no magnetic influence)

LITERATUR

1. S. Heft. Mathematische Modellierung und numerische Simulation von Kristallschmelzeströmungen unter Einbeziehung von Magnetfeldern. *Diploma thesis*, TU Berlin, 2010.
2. G. Bärwolff. Numerische Berechnung von Transportprozessen fluider Medien. *Report des Zentrums für wissenschaftlichen Gerätebau der Akademie der Wissenschaften der DDR*, Berlin, 1988.
3. G. Bärwolff and M. Hinze. Optimization of semiconductor melts. *ZAMM*, 86, (2006) 6
4. M. Gunzburger, E. Ozugurlu, J. Turner and H. Zhang. Controlling transport phenomena in the Czochralski crystal growth process. *Journal of Crystal Growth*, 234, 2002

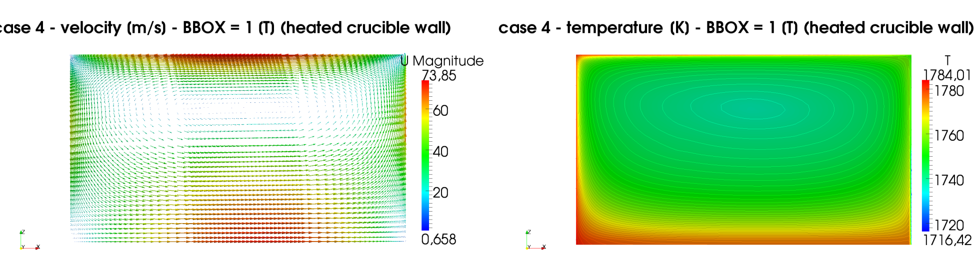

Abbildung 7. Results of numerical simulations with a heated boundary of the crucible and an initialization of the *BBoxes* with 1 *Tesla*