Crystal melt modeling and simulation with magnetic fields

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Zusammenfassung. An aspect of recent developments in crystal growth technologies is the control of electric conductive fluids by magnetic 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 consisting 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 develop and discuss the mathematical model and the numerical solution method and demonstrate some simulation results for the two-dimensional and three-dimensional case. Finally on this base an outlook for a possible benefit of the considered mathematical model and its numerical solution for a flow/melt control is given.

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THE DESCRIPTION OF THE METHOD

Firstly we concentrate ourselves on the different model stages. The Fig. ?? shows the geometrical situation.

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

\[ \nabla \cdot \mathbf{u} = 0 \quad (1) \]
\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla \mathbf{u} + \frac{1}{\rho_0} \nabla p + (1 - \beta(T - T_0)) \mathbf{g} + \frac{\alpha}{\rho_0 \mu} (\nabla \times \mathbf{B}) \times \mathbf{B} \quad (2) \]
\[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = D_T \Delta T \quad (3) \]
\[ \frac{\partial \mathbf{B}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{B} - (\mathbf{B} \cdot \nabla) \mathbf{u} = \frac{1}{\mu \sigma} \Delta \mathbf{B} \quad (4) \]

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 \( \Omega_c \).
\( \mathbf{B} \) is the magnetic flux density field which lives in the whole cylindrical model region \( \Omega_g \).

We differ the model stages

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

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

(m3) flow in the crucible coupled with the induced magnetic field (equations (??), (??), (??) in the crucible \( \Omega_c \), equation (??) in \( \Omega_g \), 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 to create a small wedge (s. Fig. ??).

![wedge geometry to describe an axi symmetric problem](image)

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 \( \Omega_c \) is a subset of the FV grid of the whole cylindrical model region \( \Omega_g \). As a source for the magnetic field we prescribe the magnetic flux density on coils in \( \Omega_g \). On the outer boundary of \( \Omega_g \) 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 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 \( \Omega_c \) with the magnetic field is realized in two steps:

1. the computation of the magnetic flux density in \( \Omega_g \) 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 \( \Omega_c \).
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. ??.

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)

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