Optimization of a thermal coupled flow problem

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Abstract: In this paper an optimization problem for a Boussinesq equation system will be formulated. To approach a given velocity field we are looking for an appropriate temperature profile on the boundary of the considered region of the thermal coupled flow problem. For a tracking type minimization functional the evaluation of the first order necessary optimality condition leads to an optimality system consisting of the forward and adjoint mathematical model.
The optimization concept will be applicated to a crystal growth flow and results of twodimensional and threedimensional model problems will be presented.

Key-Words: Free and forced convection, Boussinesq approximation, optimization of partial differential equations, crystal melt flow

1. Introduction - Motivation

During the growth of crystals crystal defects were observed under some conditions of the growth device. A transition from the twodimensional flow regime of a crystal melt in axisymmetric zone melting devices to an unsteady threedimensional behavior of the velocity and temperature field was found experimentally. This behavior leads to striations as undesirable crystal defects. To avoid such crystal defects it is important to know the parameters, which guarantee a stable steady twodimensional melt flow during the growth process.
There are several possibilities for parameter finding. In this paper optimization problems will be discussed. From the experiment and the practical crystal production process it is known that an unsteady behavior of the melt and vorticies near the fluid-solid-interphase decrease the crystal quality. Thus it makes sense to look for example for

(i) flows, which are nearly steady and

(ii) flows, which have only a small vorticity in a certain region of the melt zone.

This leads to tracking type optimization problems (i) with functionals like

$$J(\vec{u},\theta_c) = \frac{1}{2}\int_0^T \int_\Omega |\vec{u}-\overline{\vec{u}}|^2 \, d\Omega dt + \frac{\alpha}{2}\int_0^T \int_{\Gamma_c} (\theta_c^2 + \theta_{c_t}^2)\, d\Omega dt \qquad (1)$$

and problems with optimization functionals of the form

$$J(\vec{u},\theta_c) = \frac{1}{2}\int_0^T \int_\Omega |curl\vec{u}|^2 \, d\Omega dt + \frac{\alpha}{2}\int_0^T \int_{\Gamma_c} (\theta_c^2 + \theta_{c_t}^2)\, d\Omega dt \; . \qquad (2)$$

$\vec{u}$ is the velocity vector field in the melt and $\overline{\vec{u}}$ is a desired state, which represents a physically favourable flow situation. θ_c is the control temperature on the control boundary Γ_c. The discussed methods of deriving optimization and the iterative algorithms of the evaluation of necessary optimality conditions are investigated by the solution of typical crystal growth problems. Because of the difficulties to construct or to prescribe desirable flow fields we use $\overline{\vec{u}}$ which we got by a certain forward solution of the Boussinesq equation system or we set $\overline{\vec{u}}$ equal to zero. But with the optimization strategy we are ready to compute an optimal control for a given desirable flow field $\overline{\vec{u}}$ by crystal growth engineers.

2. Mathematical model

The crystal melt is described by the Navier-Stokes equations for an incompressible fluid using the Boussinesq approximation coupled with the convective heat conduction equation and the diffusion equation. Heat conductivity and viscosity depend on the temperature. Thus we have a Boussinesq equation system for the velocity $\vec{u} = (u, v, w)$, the pressure p and the temperature θ

$$\vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g} = 0, \quad (3)$$

$$-div\ \vec{u} = 0, \quad (4)$$

$$\theta_t + \vec{u} \cdot \nabla\theta - \frac{1}{Pr}\Delta\theta - f = 0\,, \quad (5)$$

on the space-time cylinder $\Omega_T = \Omega \times (0, T)$. The vector $\vec{g}$ is directed in the z-direction, i.e. $\vec{g} = (0, 0, 1)$. We will now discuss the case $f = 0$ because we are mainly interested in boundary control. $\vec{u}$ is the velocity vector. u, v, w and p are the primitive variables of the velocity vector and the pressure, ρ and θ denote the density and the temperature, Gr is the Grashof number, Pr is the Prandtl number, and f stands for an energy source.

The boundary conditions are of the form

$$\begin{aligned} &u = u_d,\ v = v_d,\ w = w_d \quad \text{on } \Gamma_T, \\ &\theta = \theta_c \quad \text{on the control boundary } \Gamma_{cT}, \\ &\theta = \theta_d, \quad \text{on } \Gamma_d \times [0, T]\,, \end{aligned} \quad (6)$$

where Γ_T means the boundary-time cylinder $\Gamma \times [0, T]$.

Dirichlet data on the control boundary as a first choice are used, because there are some results of Kurz [3], who solved an inverse problem to find a heating strategy for catching a given temperature profile on the boundary. Our idea is to find optimal temperature profiles during the optimization method, described in this paper. And after that the heater identification method of Kurz/Müller [4] can be used to find the optimal heating strategy.

In the case of the Czochralski crystal growth technique with u_d, v_d, w_d we have the possibility to describe a certain crystal and crucible rotation. In the case of zone melting flow u_d equals zero. The initial state is assumed as the neutral position of the crystal melt ($\vec{v} = \mathbf{0}$) and a temperature field, which solves the non convective heat conduction equation with the boundary conditions $\theta = \theta_d$ on Γ_d and $\theta = \theta_0$ on Γ_c. The material properties and the dimensionless parameters for the investigated crystals close the initial boundary value problem for the description of the melt flow.

3. Optimization

For the calculus of optimization and the derivation of an optimality system we use the above desrcibed dimensionless mathematical model (3), (5) with the boundary conditions (6). For $t = 0$ we have the initial condition $\vec{u} = \mathbf{0}$ and a temperature field, which solves the non convective heat conduction equation with the given temperature boundary conditions $\theta = \theta_0$ on Ω.

The use of formal Lagrange parameter technique with respect to the functional of type (1) means the consideration of the Lagrange functional

$$\begin{aligned} L(\vec{u}, p, \theta, \theta_c, \vec{\mu}, \xi, \kappa, \chi) &= J(\vec{u}, \theta_c) \\ &+ <\vec{\mu}, mo>_{\Omega_T} - <\xi, div\,\vec{u}>_{\Omega_T} \\ &+ <\kappa, en>_{\Omega_T} + <\chi, \theta - \theta_c>_{\Gamma_{cT}}\,. \end{aligned} \quad (7)$$

mo and en stand for the left sides of the equations (3) and (5), and for example for $<\vec{\mu}, mo>_{\Omega_T}$ we have

$$<\vec{\mu}, mo>_{\Omega_T} = \int_{\Omega_T} [\vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g}] \cdot \vec{\mu}\, d\Omega_T.$$

$\vec{\mu}$, ξ, κ and χ are Lagrange parameters. We will not discuss the functional analytical aspects of the used Lagrange method, i.e. function spaces, smoothness properties etc. in detail. A very good overview over the functional analytical background and the foundation of the optimization of Navier-Stokes problems is developed in [2].
To find candidates $\vec{u}(\theta_c)$ and θ_c, which minimize the functional (1) we have to analyze the necessary optimality conditions

$$L_{\vec{u}}\tilde{\vec{u}} = J_{\vec{u}}\tilde{\vec{u}} + <\vec{\mu}, mo_{\vec{u}}>_{\Omega_T} - <\xi, div\,\tilde{\vec{u}}>_{\Omega_T} + <\kappa, en_{\vec{u}}>_{\Omega_T} = 0, \quad (8)$$

$$L_p\tilde{p} = <\nabla\tilde{p}, \vec{\mu}>_{\Omega_T} = 0, \quad (9)$$

$$L_\theta\tilde{\theta} = <-Gr\,\vec{g}\,\tilde{\theta}, \vec{\mu}>_{\Omega_T} + <\kappa, en_\theta>_{\Omega_T} + <\chi, \tilde{\theta}>_{\Gamma_{cT}} = 0, \quad (10)$$

$$L_{\theta_c}\tilde{\theta_c} = J_{\theta_c}\tilde{\theta_c} + <-\chi, \tilde{\theta_c}>_{\Gamma_{cT}} = 0\,. \quad (11)$$

The derivatives of the Lagrange functional (7) to the Lagrange parameters $\vec{\mu}, \xi, \kappa, \chi$ and the necessary condition

$$\text{grad}\, L = (L_{\vec{\mu}}\tilde{\vec{\mu}}, L_\xi\tilde{\xi}, L_\kappa\tilde{\kappa}, L_\chi\tilde{\chi})^T = \mathbf{0} \quad (12)$$

means the constraints of the optimization problem, i.e. the initial boundary value problem (3),(4),(5),(6). The evaluation of the condition (8), which was described in detail in [8] leads to the following equations, boundary and final conditions for the adjoint variables. For the adjoint velocity we get from the condition (8)

$$-\vec{\mu}_t - \Delta\vec{\mu} + (\nabla\vec{u})^t\vec{\mu} - (\vec{u}\cdot\nabla)\vec{\mu} + \nabla\xi + \kappa\nabla\theta = -(\vec{u} - \overline{\vec{u}}) \quad \text{in} \quad \Omega_T\,, \quad (13)$$

with the boundary condition $\vec{\mu} = \mathbf{0}$ on $\Gamma \times (0,T)$, and the final condition $\vec{\mu}(T) = \mathbf{0}$ in Ω. Equation (9) yields

$$-div\,\vec{\mu} = 0 \quad \text{in} \quad \Omega_T\,. \quad (14)$$

The condition (10) implies

$$-\kappa_t - \frac{1}{Pr}\Delta\kappa - \vec{u}\cdot\nabla\kappa = Gr\,\vec{g}\cdot\vec{\mu} \quad \text{in} \quad \Omega_T\,, \quad (15)$$

with the boundary condition $\kappa = 0$ on $\Gamma \times (0,T)$, and the final condition $\kappa(T) = 0$ in Ω, and the choice of χ as

$$\chi = -\frac{1}{Pr}\frac{\partial\kappa}{\partial\mathbf{n}} \quad \text{on} \quad \Gamma_{cT}\,.$$

Condition (11) gives

$$\alpha(-\theta_{c_{tt}} + \theta_c) = \chi\ (= -\frac{1}{Pr}\frac{\partial\kappa}{\partial\mathbf{n}}) \quad \text{on} \quad \Gamma_{cT}\,, \quad (16)$$

with the time boundary conditions

$$\theta_c(0) = \theta_0 \quad \text{and} \quad \theta_{c_t}(T) = 0\,, \quad (17)$$

where θ_0 means a temperature distribution on Γ_c at the beginning of the melting process, which is physical and technological founded. Now we can summarize, and the fully optimization system consists of

1) the forward model with the Boussinesq equations (3),(4),(5), the boundary condition (6) and the given initial state for the velocity field $\vec{u}$, the pressure p and the temperature θ, and
2) the adjoint model with the equations (13),(14),(15),(16), and the boundary and final conditions for the adjoint variables $\vec{\mu}$, ξ, κ and the control θ_c,

and we will call it the optimality system. The global existence of a solution of the forward problem is well known [5]). In three dimensions only the local uniqueness of the forward solution could be shown. Hinze/Kunisch [2] have shown the existence and uniqueness of a solution of the adjoint model. Minimization functionals of the considered types (1) are investigated for example by Hinze [2]and Gunzburger et al. [6]. The main reason for such quadratic functionals is the technological aim of the crystal growth methods. This purpose dominates qualitativ mathematical questions - for example like existence of a minimum - which are still under consideration.

4. To the numerical solution method of the full problem

Now we construct a numerical solution method. The used time discretization should be demonstrated for the forward problem (3)-(6), i.e. the boussinesq equation system. Quantities without upper indices are considered at the old time level $t_n = n\tau$ with the time step τ. The upper index $n+1$ indicates the values at the new time level $t_{n+1} = (n+1)\tau$. With $\tau = \frac{T}{Z}$ we have a discretization $t_0 = 0$, $t_1 = \tau$, $t_2 = 2\tau, \ldots, t_Z = Z\tau = T$

of the considered time intervall $[0,T]$. We use an implicit time discretization related to the conductive terms. Thus we have in the time-space cylinder Ω_T the time integration scheme

$$\frac{\vec{u}^{n+1}-\vec{u}}{\tau}+(\vec{u}\cdot\nabla)\vec{u}-\Delta\vec{u}^{n+1}+\nabla p^{n+1} \\ -Gr\,\theta^{n+1}\vec{g}=0 \quad (18)$$

$$-div\ \vec{u}^{n+1}=0 \quad (19)$$

$$\frac{\theta^{n+1}-\theta}{\tau}+(\vec{u}\cdot\nabla)\theta-\frac{1}{Pr}\Delta\theta^{n+1}=0\ . \quad (20)$$

The divergence of the equation (18) gives

$$-\Delta p^{n+1}=-\frac{1}{\tau}div\ \vec{\hat{u}} \quad , \quad (21)$$

with

$$\vec{\hat{u}}=\vec{u}+\tau[(\vec{u}\cdot\nabla)\vec{u}+Gr\,\theta^{n+1}\vec{g}]\ . \quad (22)$$

With the solution p^{n+1} of the equation (21) the velocity field $\vec{u}^{n+1}$ we get as the solution of

$$\frac{1}{\tau}\vec{u}^{n+1}-\Delta\vec{u}^{n+1}=\frac{1}{\tau}\vec{u}-\nabla p^{n+1} \quad . \quad (23)$$

The used time discretization means the solution of a Poisson equation for p^{n+1}, four Helmholtz equations for the components of $\vec{u}^{n+1}$ and θ^{n+1}. The spatial finite volume discretization developed in [1] of the equations (21), (23) and (20) leads to linear equation systems with symmetric coefficient matrices which we solve with conjugate gradient methods.

For the solution of the adjoint problem we use the following time discretization, which was developed in detail in [8].

$$\frac{\vec{\mu}^{n-1}-\vec{\mu}}{\tau}-\Delta\vec{\mu}^{n-1}+(\nabla\vec{u}^{n-1})^t\vec{\mu} \\ -(\vec{u}^{n-1}\cdot\nabla)\vec{\mu}+\nabla\xi \\ =-(\vec{u}^{n-1}-\overline{\vec{u}})-\kappa^{n-1}\nabla\theta, \quad (24)$$

$$-div\ \vec{\mu}^{n-1}=0, \quad (25)$$

$$\frac{\kappa^{n-1}-\kappa}{\tau}-\vec{u}^{n-1}\cdot\nabla\kappa-\frac{1}{Pr}\Delta\kappa^{n-1} \\ =Gr\,\vec{g}\cdot\vec{\mu} \quad (26)$$

in the time-space cylinder Ω_T. The equation (16) for the control with the boundary conditions $\theta_c(\gamma,0)=\theta_{c0}$ and $\theta_{c_t}(\gamma,T)=0$ for $\gamma\in\Gamma_c$ will be solved with a finite volume method in space and time. The solution of the discretized system (3)-(6) and (13)-(17) is difficult and expensive, because of the opposite time direction of the forward system (3)-(6) and the adjoint system (13)-(17). That means we have to provide the forward solution $\vec{u},\theta$ on the whole time interval $[0,T]$ to get the adjoint solution $\vec{\mu},\kappa,\theta_c$ and vice versa.

If we have discretized the time interval $[0,T]$ by Z timesteps $\tau=\frac{1}{Z}$ and the dimensions of the spatial discretizations are N, M and P a direct solution of the whole system means the solution of an algebraic equation system with $2Z\times N\times M\times P\times 10$ equations. For the representation of the used iteration method we denote with $\mathcal{H}:=-\partial_{tt}+id$ a solution operator, which describes the solution of the two point boundary value problem (16),(17) on Γ_{cT}, i.e.

$$\mathcal{H}(\theta_c)=\chi \quad \text{or} \quad \theta_c=\mathcal{H}^{-1}(\chi)\ .$$

Iterative methods of the form

i) choose a suitable start value of θ_c,

ii) solve the forward problem and get $[\vec{u},\theta](\theta_c)$

iii) solve the adjoint problem and get $[\vec{\mu},\kappa](\vec{u},\theta)$
update of θ_c by $\theta_c:=\sigma_r\theta_c+(1-\sigma_r)\mathcal{H}^{-1}(\chi)$, $\sigma_r\in]0,1[$,

iv) until convergence, go to ii),

are used. During one time step of the forward problem we have to solve equations of the type (21), a Poisson equation, and with (23),(20) four Helmholtz equations (for the adjoint problem also five equations of the same type). The above described fixpoint iteration i)-iv) with relaxation works good, and the results of the numerical simulations will be demonstrated now.

5. Results of the numerical solution of the full problem

As a testproblem we consider a zone melting configuration. The used geometrical and material parameters for the crystal $(Bi_{0.25}Sb_{0.75})_2Te_2$, a composition of bismuth point fifty antimony one point fifty telurium two, are summarized in the table 1 (see also [1]).

$(Bi_{0.25}Sb_{0.75})_2Te_2$-crystals are used for small cooling devices. The figure 1 shows the physical domain of the melt zone. For the velocity we have homogeneous dirichlet data on the whole boundary. For the temperature we have the boundary conditions

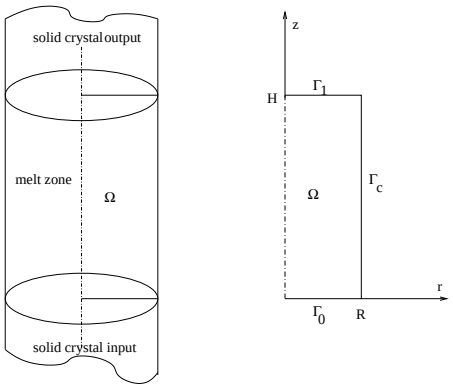

Figure 1: Physical domain for the zone melting growth

$$\theta = \theta_c, \text{ for } r = R, 0 \le z \le H, \varphi \in (0, 2\pi), \quad (27)$$
$$\theta = \theta_s, \text{ for } 0 \le r \le R, z = H, \quad (28)$$
$$\theta = \theta_s, \text{ for } 0 \le r \le R, z = 0. \quad (29)$$

For $t = 0$ we start with a given temperature profile $\theta_c = \theta_{c0}$ on Γ_c and with $\theta_s = 613\,K$, $\delta\theta = 25\,K$ for θ_{c0} we have

$$\theta_{c0}(z) = \theta_s + 4\frac{z}{H}(1 - \frac{z}{H})\delta\theta \ .$$

The velocity field $\overline{\vec{u}}$, which we want to reach is

parameter	symbol	value
radius	R	0.004 m
height	H	0.016 m
melting point	θ_s	613 K
diffusivity	a	0.44000e-05 $\frac{m^2}{s}$
viscosity	ν	0.36310e-06 $\frac{m^2}{s}$
expansion	β	0.96000e-04 K^{-1}

Table 1: Parameters of $(Bi_{0.25}Sb_{0.75})_2Te_2$-melt and of the melt geometry

a) a typical twodimensional toroidal flow and b) a non moving melt $\overline{\vec{u}} = \mathbf{0}$.

The case b) is artificial but a good test case because we knew that $\theta_c = \theta_s = const.$ gives $\vec{u} = \mathbf{0}$ and $\theta = \theta_s$ as a solution of the boussinesq equation system. We consider a time interval $[0, T] = [0, 8\,\text{seconds}]$ with $Z = 60$ time steps of 0.1222 seconds. For the spatial discretization we use 20×30 finite volumes. The figures 2 - 4 show the results of the optimization for the case a) and case b), i.e. the resulting control temperature on the boundary-time cylinder and the development of the functional values, where the temperatures are dimensionless defined by $\bar{\theta} = \frac{\theta - \theta_s}{\delta}$.

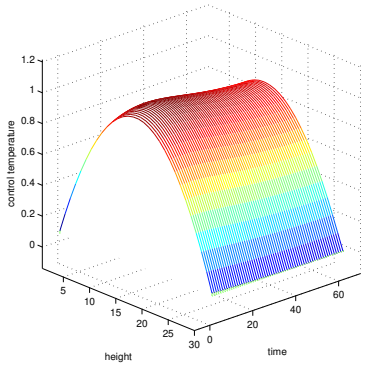

Figure 2: Control temperature (problem a)

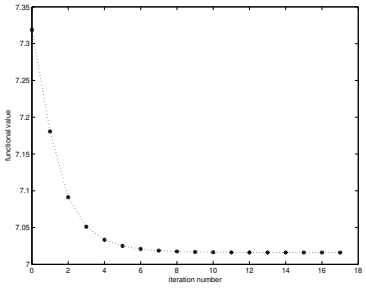

Figure 3: Functional vs. iteration (problem a)

6. Conclusion

With the Lagrange parameter technique it's possible to derive an optimization system for a given functional, which solution gives an

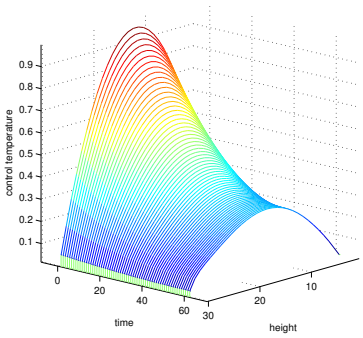

Figure 4: Control temperature (problem b)

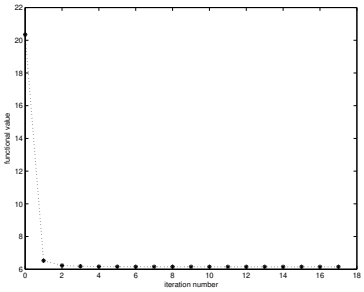

Figure 5: Functional vs. iteration (problem b)

optimal control. The numerical examples of the fully time-depend 2.5d optimization system show the possibility of the practical optimization of a thermal coupled flow problem in the crystal growth field. The results show the possibility of boundary control especially in the case of the zone melting technique. Based on the results the proposed strategies it is now possible to do a fully 3d optimization. For the Czochralski growth configuration the optimization works, but the results show, that these kind of boundary control is not really of practical interest.

It is necessary to continue numerical experiments to investigate if the optimization during a boundary control only will be successful technology. There are some experiences with other optimization problems which show the efficiency of volume control, if there is a possibility of the production of volume forces (for example by a magnetic field).

The presented optimization method is applicable to other coupled transport problems for example the coupling of solutal and natural convection. The demonstrated derivation of the adjoint problem to fit the necessary optimality condition $\operatorname{grad} L = \mathbf{0}$ (L denotes the Lagrange function including the differential equations and the minimization functional) is the key to process optimization with infinite degrees of freedom.

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