Two- and Threedimensional Flow Optimization in Chemical Engineering

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1 Introduction

In several mathematical models of engineeering processes the Boussinesq equation system occurs. Especially for melting processes the heating by the realisation of certain boundary conditions is responsible for the resulting flow and temperature field. Beside the thermal boundary conditions non homogeneous velocity boundary conditions influence also the melt flow. Thus the control of certain boundary conditions is a possibility to optimize the process with the aim of reaching flow and temperature fields which guarantee desirable results of the melting process.
We will discuss this optimization with partial differential equations for the problem of crystal melts with the aim of having single crystals without defects in the result of the melting process.
This leads to tracking type optimization problems with a functional like

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

$\boldsymbol{u}$ is the velocity vector field in the melt and $\overline{\boldsymbol{u}}$ is the state, which we want to have, θ_c is the control temperature on the control boundary Γ_c.

2 Mathematical model

The crystal melt is described by the Navier-Stokes equation 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. Because of the axisymmetric situation of the melting zone we write down the equations in cylindical coordinates. Thus we have a Boussinesq equation system in cylindrical coordinates for the velocity $\boldsymbol{u} = (u, v, w)$, the pressure p and the temperature θ.
For the velocity no slip boundary conditions are used. But in the case of rotating crystals and crucibles we have in the circumferential direction inhomogeneous velocity boundary conditions given by rotation numbers. At the interfaces between the solid material and the fluid crystal melt we have for the temperature inhomogeneous Dirichlet data, i.e. the melting point temperature. On the heated coat (control boundary) of the ampulla the experimentators gave us measured

temperatures and we will look further for optimal profiles during the optimization. The initial state was assumed as the neutral position of the crystal melt ($\boldsymbol{v} = \mathbf{0}$) and a temperature field, which solves the non convective heat conduction equation with the given temperature boundary conditions. The material properties and the dimensionless parameters for the investigated crystal 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 optimization system we start with the Boussinesq equation system for the velocity vector $\boldsymbol{u}$ and the temperature θ in the space time cylinder $\Omega_T = \Omega \times (0,T)$. For the boundary conditions we have

$$\boldsymbol{u} = \boldsymbol{u}_g \quad \text{on } \Gamma \times (0,T), \quad \theta = \theta_c \quad \text{on } \Gamma_{cT}, \quad \text{and} \quad \theta = 0 \quad \text{on } \Gamma_d \times (0,T), \tag{2}$$

where Γ is the boundary of the spatial region $\Omega \subset \mathbb{R}^3$, on which the problem lives, and Γ_c is the control boundary, Γ_d is the Dirichlet part of the boundary and $\Gamma_{cT} = \Gamma_c \times (0,T)$. That means in this paper our interest is focussed on the temperature boundary control. For $t = 0$ we have the initial condition $\boldsymbol{u} = \mathbf{0}$ 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 parameters technique with respect to the functional of type (1) means the consideration of the Langrange functional

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

mo and *en* stand for the left sides of the impulse and energy balance. The Lagrange functional means the objective of the optimization

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

the restrictions i.e. the weak formulation of the occuring partial differential equations

$$\begin{aligned} < \boldsymbol{\mu}, mo >_{\Omega_T} &= \int_{\Omega_T} [\boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \Delta \boldsymbol{u} + \nabla p - \rho(\theta)\boldsymbol{g}] \cdot \boldsymbol{\mu} \, d\Omega \, dt \, , \\ < \xi, div\, \boldsymbol{u} >_{\Omega_T} &= \int_{\Omega_T} \xi \, div\, \boldsymbol{u} \, d\Omega dt \, , \\ < \kappa, en >_{\Omega_T} &= \int_{\Omega_T} [\theta_t + \boldsymbol{u} \cdot \nabla \theta - \frac{1}{Pr} \Delta \theta] \, \kappa \, d\Omega dt \, , \end{aligned}$$

and the condition for the boundary control

$$< \chi, \theta - \theta_c >_{\Gamma_{cT}} = \int_{\Gamma_{cT}} [\theta - \theta_c] \, \chi \, d\Gamma dt \, ,$$

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

$$\begin{aligned}
L_{\boldsymbol{u}}\tilde{u} &= J_{\boldsymbol{u}}\tilde{u} + <\boldsymbol{\mu}, mo_{\boldsymbol{u}}>_{\Omega_T} - <\xi, div\tilde{u}>_{\Omega_T} + <\kappa, en_{\boldsymbol{u}}>_{\Omega_T} = 0,\\
L_p\tilde{p} &= <\nabla\tilde{p}, \boldsymbol{\mu}>_{\Omega_T} = 0,\\
L_\theta\tilde{\theta} &= <-\rho_\theta \boldsymbol{g}\tilde{\theta}, \boldsymbol{\mu}>_{\Omega_T} + <\kappa, en_\theta>_{\Omega_T} + <\chi, \tilde{\theta}>_{\Gamma_{cT}} = 0,\\
L_{\theta_c}\tilde{\theta_c} &= J_{\theta_c}\tilde{\theta_c} + <-\chi, \tilde{\theta_c}>_{\Gamma_{cT}} = 0\ ,
\end{aligned}$$

i.e. the Frechet derivative of the Lagrange functional equal to zero. The evaluation of the necessary optimality condition gives the equation for the adjoint velocity

$$-\boldsymbol{\mu}_t - \Delta\boldsymbol{\mu} + (\nabla\boldsymbol{u})^t\boldsymbol{\mu} - (\boldsymbol{u}\cdot\nabla)\boldsymbol{\mu} + \nabla\xi = -(\boldsymbol{u} - \overline{\boldsymbol{u}}) - \kappa\nabla\theta \quad \text{in} \quad \Omega_T\ , \tag{3}$$

with the boundary condition and the final condition

$$\boldsymbol{\mu} = \boldsymbol{0} \quad \text{on} \quad \Gamma\times(0,T), \quad \text{and} \quad \boldsymbol{\mu}(T) = \boldsymbol{0} \quad \text{in} \quad \Omega\ , \tag{4}$$

and the equation

$$-div\ \boldsymbol{\mu} = 0 \quad \text{in} \quad \Omega_T\ . \tag{5}$$

For the adjoint temperature κ we get

$$-\kappa_t - \frac{1}{Pr}\Delta\kappa - (\boldsymbol{u}\cdot\nabla)\kappa = -\rho_\theta\boldsymbol{g}\cdot\boldsymbol{\mu} \quad \text{in} \quad \Omega_T\ , \tag{6}$$

with the boundary condition and the final condition

$$\kappa = 0 \quad \text{on} \quad \Gamma\times(0,T)\ , \quad \text{and} \quad \kappa(T) = 0 \quad \text{in} \quad \Omega\ , \tag{7}$$

and with the choice of the free χ as $\chi = \frac{1}{Pr}\frac{\partial\kappa}{\partial\mathbf{n}}$ on Γ_{cT} we get for the control the equation

$$-\theta_{c_{tt}} + \theta_c = \frac{1}{Pr}\frac{\partial\kappa}{\partial\mathbf{n}} \quad \text{on} \quad \Gamma_{cT}\ , \tag{8}$$

with the time boundary conditions

$$\theta_{c_t}(0) = \theta_{c_t}(T) = 0\ . \tag{9}$$

The optimality system consists of the forward model with the Boussinesq equation system and the boundary conditions (2) and the given initial state for the velocity field $\boldsymbol{u}$, the pressure p and the temperature θ, and the adjoint model with the equations (3),(5),(6),(8), and the conditions (4),(7),(9) for the adjoint variables $\boldsymbol{\mu}$, ξ, κ and the control θ_c.

4 To the numerical solution method

The optimization system is now under consideration for a numerical solution. The Boussinesq equation system is solved with a finite volume method [1]. In the present case of axisymmetric conditions we can transform the adjoint equations into a cylindrical coordinate system. Using the adjoint divergence condition $div\ \boldsymbol{\mu} = 0$ we can write the adjoint equations in the following quasi conservative form. For adjoint velocity $\boldsymbol{\mu} = (\mu, \nu, \omega)$ in the cylindrical coordinate system with the radial component μ, the azimuthal component ν and the z-component ω we get from (3) for example for μ

$$\begin{aligned} &-\mu_t - ((r\mu)_r/r)_r - \mu_{\varphi\varphi}/r^2 + 2\mu_\varphi/r^2 - \mu_{zz} + \mu u_r + \nu v_r + \omega w_r \\ &-(ru\mu)_r/r - (v\mu)_\varphi/r - (w\mu)_z + v\nu/r + \xi_r = -(u - \overline{u}) - \kappa\theta_r\ . \end{aligned} \tag{10}$$

From equation (6) we get for the adjoint temperature κ

$$-\kappa_t - \frac{1}{Pr}[(r\kappa_r)_r/r + \kappa_{\varphi\varphi}/r^2 + \kappa_{zz}] - (ru\kappa)_r/r - (v\kappa)_\varphi/r - (w\kappa)_z = -\rho_\theta g w\ . \tag{11}$$

Equation (11) is a convective heat conduction equation and the discretization can be done like those in [1]. In the equation (10) and the equations for ν, ω the terms $(\nabla \boldsymbol{u})^t \boldsymbol{\mu}$ and $\kappa \nabla \theta$ are not known from the classical Navier-Stokes equations and they will by discretized in a canonical way for staggered grids. The solution of the discretized Boussinesq equation system and the equations for ν, ω and ξ (3) is difficult and expensive, because of the opposite time direction of the forward system and the adjoint system. That means we know the forward solution $\boldsymbol{u}, \theta$ on the whole time interval $[0, T]$ to get the adjoint solution $\boldsymbol{\mu}, \kappa$ and vice versa. If we have discretized the time interval $[0, T]$ by Z timesteps 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. Iterative methods of the form

i) choose a suitable start value of $\boldsymbol{u}, \theta$,
ii) solve the adjoint problem and get $[\boldsymbol{\mu}, \kappa, \theta_c](\boldsymbol{u}, \theta)$
iii) solve the forward problem and get $[\boldsymbol{u}, \theta](\theta_c)$
iv) until convergence, go to ii),

are realized and we will now discuss the results of the proposed method.

5 Results of the optimzation

In the table 1 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 ([1]). We consider the temperature boundary control of the the zone melting method. The melting zone (integration region Ω) is shown in figure 1. For the temperature we have the boundary conditions

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

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

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

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 $\overline{\boldsymbol{u}}$, which we want to reach is a typical twodimensional toroidal flow and We consider a time interval $[0, T] = [0, 4\,\text{seconds}]$ with $Z = 60$ time steps of 0.0661 seconds. For the spatial discretization we use 20×25 finite volumes. The figures 2 and 3 show the result of the optimization. As a threedimensional testproblem we consider the above discussed zone melting configuration. The aim of the optimization is to reach a velocity field $\overline{\mathbf{u}} = \mathbf{0}$. This an artificial but a good test case. The size of the spatial discretization of $[0, 2\pi]x[0, R]x[0, H]$ is $20 \times 20 \times 30$. We consider the time interval $[0, T] = [0, 4\,\text{seconds}]$ with $Z = 60$ time steps of 0.0661 seconds. The figure 4 shows the control temperature $\theta_c(\varphi, z)$ at the time $t = T$ on Γ_c and the development of the functional values during The figures 4 shows the twodimensionality of the control temperature θ_c, which does not depend on the angle φ.

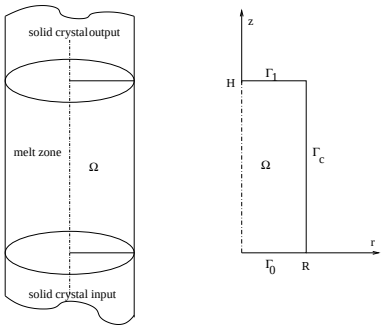

Fig. 1. Physical domain for the zone melting growth

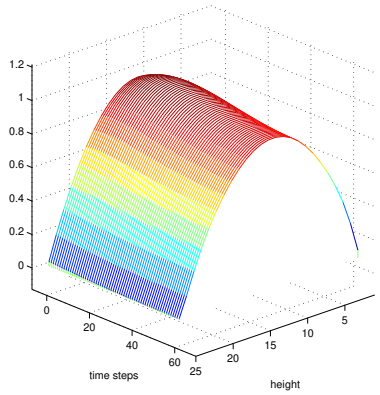

Fig. 2. control on the boundary time cylinder

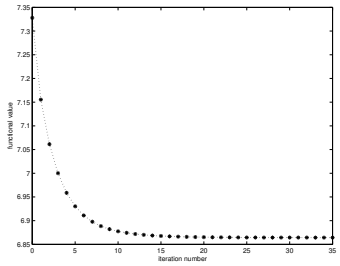

Fig. 3. decreasing functional values during the fixpoint iteration

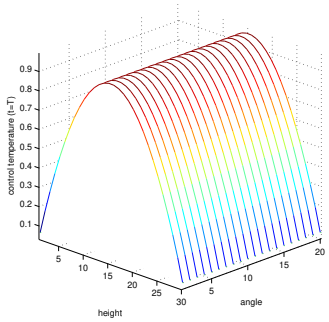

Fig. 4. optimal control in the 3d case

6 Conclusion

With the Lagrange parameter technique it's possible to derive an optimization system for a given functional, which solution gives an optimal control. The numerical examples of the complete 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. 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).

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