Iranian Journal of Operations Research
Vol. 10, No. 2, 2019, pp. 40-48

Optimization of A Thermal Coupled Flow Problem of Semiconductor Melts

G. Bärwolff [1]

In this paper we describe the formal Lagrange-technique to optimize the production process of solid state crystals from a mixture crystal melt. After the construction of the adjoint equation system of the Boussinesq equation of the crystal melt the forward and backward problems (KKT-system) are discretized by a conservative finite volume method.

***Keywords**: Mathematical model of crystal melt, Boussinesq equation system, Necessary optimality conditions, Adjoint problem, Numerical solution*.

Manuscript was received on 01/09/2019, revised on 10/11/2019 and accepted for publication on 18/12/2019.

1. Introduction

During the growth of crystals crystal defects are observed under some conditions of the growth device. As a result of experiments, a transition from the two dimensional flow regime of a crystal melt in cylinder-symmetric zone melting devices to an unsteady three dimensional behavior of the velocity and temperature field is 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 two dimensional 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-inter-phase decreases 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 with functionals like

$$J(\mathbf{u}, \theta_c) = \frac{1}{2}\int_0^T \int_\Omega |\mathbf{u} - \bar{\mathbf{u}}|^2 d\Omega dt + \frac{1}{2}\int_0^T \int_{\Gamma_c} \left(\theta_c^2 + \theta_{c_t}^2\right) d\Omega dt, \tag{1}$$

and problems with optimization functionals of the form

[1] Department of Mathematics, Technical University of Berlin, Berlin, Germany, Email: baerwolf@math.tu-berlin.de.

$$J(\mathbf{u},\theta_c) = \frac{1}{2}\int_0^T \int_\Omega |curl\ \mathbf{u}|^2 d\Omega dt + \frac{1}{2}\int_0^T \int_{\Gamma_c} \theta_c^2\ d\Omega dt, \tag{2}$$

where $\mathbf{u}$ is the velocity vector field in the melt and $\bar{\mathbf{u}}$ is the state, which we want to have, and θ_c is the control temperature on the control boundary Γ_c. The melt flow is described by the Navier-Stokes equation with the Boussinesq-approximation for the influence of natural convection coupled with the convective heat conduction equation. In addition to the thermal effects, the solutal convection can be considered optional by a diffusion equation.

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 cylinder-symmetric situation of the melting zone, we write down the equations in cylindrical coordinates. Thus, we have the governing equations,

$$u_t + (ruu)_r/r + (uv)_\varphi/r + (wu)_z - v^2/r = -p_r + ((ru)_r/r)_r + u_{\varphi\varphi}/r^2 - 2v_\varphi/r^2 + u_{zz}, \tag{3}$$

$$v_t + (ruv)_r/r + (vv)_\varphi/r + (wv)_z - uv/r = -p_\varphi/r + ((rv)_r/r)_r + v_{\varphi\varphi}/r^2 + 2u_\varphi/r^2 + v_{zz}, \tag{4}$$

$$w_t + (ruw)_r/r + (vw)_\varphi/r + (ww)_z = -p_z + (rw_r)_r/r + w_{\varphi\varphi}/r^2 + w_{zz} + \rho(\theta)g \tag{5}$$

$$(ru)_r/r + v_\varphi/r + w_z = 0, \tag{6}$$

$$\theta_t + (ru\theta)_r/r + (v\theta)_\varphi + (w\theta)_z = \frac{1}{Pr}[(r\theta_r)_r/r + \left(\theta_\varphi\right)_\varphi/r^2 + (\theta_z)_z] + q, \tag{7}$$

in the cylindrical melt zone (height H, radius R), where 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, Pr is the Prandtl number, and g is the body force and q stands for an energy source.

For the velocity, no slip boundary conditions are used. At the interfaces between the solid material and the fluid crystal melt we have for the temperature homogeneous Dirichlet data, i.e., the melting point temperature. On the heated coat of the ampoule, the experimentors gave us measured temperatures. After a homogenization, the boundary conditions are of the form

$$u = v = w = 0 \quad \text{on the whole boudary}, \tag{8}$$

$$\theta = \theta_c \quad \text{for } r = 1, \qquad 0 \le z \le 2\alpha, \varphi \in (0,2\pi), \qquad (\text{this is the control boundary } \Gamma_c) \tag{9}$$

$$\theta = 0, \qquad \text{for } 0 \le r \le 1, \qquad z = 0, \qquad z = 2\alpha, \qquad \varphi \in (0,2\pi). \tag{10}$$

The initial state was assumed as the neutral position of the crystal melt ($\mathbf{u} = \mathbf{0}$) and a temperature field, which solves the non-convective heat conduction equation with the given temperature boundary conditions.

A three-dimensional finite volume code is used for the numerical solution of the above described non-linear initial boundary value problem.

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 use the mathematical model in Cartesian coordinates, which turns to be

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \Delta\mathbf{u} + \nabla p - \rho(\theta)\vec{g} = 0 \quad \text{on } \Omega_T, \tag{11}$$

$$-div\,\mathbf{u} = 0 \quad \text{on } \Omega_T, \tag{12}$$

$$\theta_t + (\mathbf{u}\cdot\nabla)\theta - \frac{1}{Pr}\Delta\theta - q = 0 \quad \text{on } \Omega_T, \tag{13}$$

$$\mathbf{u} = 0 \quad \text{on } \Gamma_T, \tag{14}$$

$$\theta = \theta_c \quad \text{on } \Gamma_c \times (0,T), \tag{15}$$

$$\theta = 0 \quad \text{on } \Gamma_d \times (0,T), \tag{16}$$

where $\Gamma = \Gamma_c \cup \Gamma_d$ is the boundary of the spatial region $\Omega \subset \mathbb{R}^3$, on which the problem lives, $\Gamma_T = \Gamma \times (0,T)$, Γ_c is the control boundary and Γ_d is the Dirichlet part of the boundary. For $t = 0$, we have the initial condition $\mathbf{u} = \mathbf{0}$ 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 Lagrange functional

$$L(\mathbf{u},p,\theta,\theta_c,\mathbf{w},\xi,\kappa,\chi) = \\ J(\mathbf{u},\theta_c) + \langle \mathbf{w}, moment\rangle_{\Omega_T} - \langle \xi, div\,\mathbf{u}\rangle_{\Omega_T} + \langle \kappa, energy\rangle_{\Omega_T} + \langle \chi, \theta - \theta_c\rangle_{\Gamma_c\times(0,T)}, \tag{17}$$

where $moment$ and $energy$ respectively stand for the left sides of the equations (11) and (13), and for example for $\langle \mathbf{w}, moment\rangle_{\Omega_T}$ we have

$$\langle \mathbf{w}, moment\rangle_{\Omega_T} = \int_{\Omega_T} [\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \Delta\mathbf{u} + \nabla p - \rho(\theta)\vec{g}]\cdot\mathbf{w}\, d\Omega dt\,, \tag{18}$$

where $\mathbf{w}, \xi, \kappa$ and χ are Lagrange parameters, and it is cleary, that

$$L(\mathbf{u},p,\theta,\theta_c,\mathbf{w},\xi,\kappa,\chi) = J(\mathbf{u},\theta_c),$$

if $\mathbf{u}, p$ and θ comprise a solution of the above described thermal coupled boundary value problem. 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 foundation of the optimization of Navier-Stokes problems is developed in M. Hinze (2000).

To find candidates $\mathbf{u}(\theta_c)$ and θ_c, which minimize the functional (1), we need the necessary conditions:

$$L_{\mathbf{u}}\tilde{u} = J_{\mathbf{u}}\tilde{u} + \langle w, moment_{\mathbf{u}}\rangle_{\Omega_T} - \langle \xi, div\ \tilde{u}\rangle_{\Omega_T} + \langle \kappa, energy_{\mathbf{u}}\rangle_{\Omega_T} = 0, \tag{19}$$
$$L_p\tilde{p} = \langle \nabla\tilde{p}, \mathbf{w}\rangle_{\Omega_T} = 0, \tag{20}$$
$$L_\theta\tilde{\theta} = \langle -\rho_\theta\vec{g}\tilde{\theta}, \mathbf{w}\rangle_{\Omega_T} + \langle \kappa, energy_\theta\rangle_{\Omega_T} + \langle \chi, \tilde{\theta}\rangle_{\Gamma_c\times(0,T)} = 0, \tag{21}$$
$$L_{\theta_c}\tilde{\theta}_c = J_{\theta_c}\tilde{\theta}_c + \langle -\chi, \tilde{\theta}_c\rangle_{\Gamma_c\times(0,T)} = 0. \tag{22}$$

Let us have a closer look at the condition (19). For $J_{\mathbf{u}}\tilde{u}$, we find

$$J_{\mathbf{u}}\tilde{u} = \int_{\Omega_T} [\mathbf{u} - \bar{\mathbf{u}}] \cdot \tilde{u}\ d\Omega dt\ , \tag{23}$$

where term $\langle w, moment_{\mathbf{u}}\rangle_{\Omega_T}$ means the derivative of the Navier-Stokes equation, i.e.,

$$\langle \mathbf{w}, moment\rangle_{\Omega_T} = \int_{\Omega_T} [\tilde{u}_t - \Delta\tilde{u} + (\mathbf{u}\cdot\nabla)\tilde{u} + (\tilde{u}\cdot\nabla)\mathbf{u}] \cdot \mathbf{w}\ d\Omega dt, \tag{24}$$

The discussion of the term $\langle \kappa, energy_{\mathbf{u}}\rangle_{\Omega_T}$ gives

$$\langle \kappa, energy_{\mathbf{u}}\rangle_{\Omega_T} = \int_{\Omega_T} [(\tilde{u}\cdot\nabla)\theta]\ \kappa\ d\Omega dt, \tag{25}$$

Using the rules of integration by parts from (23)-(25) and (19), we get for all test vector functions $\tilde{u}$:

$$L_{\mathbf{u}}\tilde{u} = \int_{\Omega_T} [-\mathbf{w}_t - \Delta\mathbf{w} + (\nabla\mathbf{u})^t\mathbf{w} - (\mathbf{u}\cdot\nabla)\mathbf{w} + \nabla\xi + (\mathbf{u} - \bar{\mathbf{u}}) + \kappa\nabla\theta] \cdot \tilde{u}\ d\Omega dt\ = 0,$$

or

$$-\mathbf{w}_t - \Delta\mathbf{w} + (\nabla\mathbf{u})^t\mathbf{w} - (\mathbf{u}\cdot\nabla)\mathbf{w} + \nabla\xi = -(\mathbf{u} - \bar{\mathbf{u}}) - \kappa\nabla\theta \quad \text{in} \quad \Omega_T, \tag{26}$$

with the boundary condition

$$\mathbf{w} = 0 \quad \text{on} \quad \Gamma\times(0,T), \tag{27}$$

and the final condition

$$\mathbf{w}(T) = 0 \quad \text{in} \quad \Omega, \tag{28}$$

The necessary condition (20) gives for all test functions $\tilde{p}$ the equation

$$-div\ \mathbf{w} = 0 \quad \text{in} \quad \Omega_{\mathrm{T}}. \tag{29}$$

The condition (21) means

$$L_\theta \tilde{\theta} = \int_{\Omega_T} -\rho_\theta \vec{g} \cdot \mathbf{w} \tilde{\theta}\, d\Omega dt + \int_{\Omega_T} \left[\tilde{\theta}_t - \frac{1}{Pr} \Delta \tilde{\theta} + u \cdot \nabla \tilde{\theta} \right] \kappa \, d\Omega dt + \int_{\Gamma_c \times (0,T)} \chi \tilde{\theta}\, d\Gamma_c dt = 0,$$

or after the integration by parts for all test functions $\tilde{\theta}$ we get the equation

$$-\kappa_t - \frac{1}{Pr} \Delta \kappa - \mathbf{u} \cdot \nabla \kappa = -\rho_\theta \vec{g} \cdot \mathbf{w} \quad \text{in} \quad \Omega_T, \tag{30}$$

with the boundary condition

$$\kappa = 0 \quad \text{on} \quad \Gamma_T, \tag{31}$$

and the final condition

$$\kappa(T) = 0 \quad \text{in} \quad \Omega, \tag{32}$$

and the choice of χ as

$$\chi = \frac{1}{Pr} \frac{\partial \kappa}{\partial \mathbf{n}} \quad \text{on} \quad \Gamma_c \times (0, T).$$

The evaluation of the condition (22) finally gives

$$\theta_{c_{tt}} + \theta_c = \chi = \frac{1}{Pr} \frac{\partial \kappa}{\partial \mathbf{n}} \quad \text{on} \quad \Gamma_c \times (0, T), \tag{33}$$

with the time boundary conditions

$$\theta_{c_t}(0) = \theta_{c_t}(T) = 0. \tag{34}$$

Now, we can summarize and the full optimization system consists of

- the forward model with the Boussinesq equations (11), (12), (13), the boundary conditions (14), (15), (16) and the given initial state for the velocity field $\mathbf{u}$, the pressure p and the temperature θ, and

- the adjoint model with the equations (26), (29), (30), (33), the boundary conditions (27), (31), (34) and the anal conditions (28), (32) for the adjoint variables w, ξ, κ and the control θ_c.

The global existence for a solution of the forward problem is well-known; see Ladyzhenskaya (1969), Constantin, Foias (1988). In three dimensions only the local uniqueness of the forward solution could be shown. Hinze (2000) showed the existence and uniqueness of a solution of the adjoint model. For the used minimization functionals (1) and (2), Hinze has showed the positive definiteness of the Hessian $\hat{J}''(\theta_c)$ of

$$\hat{J}(\theta_c) := J(\mathbf{u}(\theta_c), \theta_c),$$

and with this result we have a sufficient second order optimality condition.

4. Optimization with Infinite Degrees of Freedom vs. Optimization of Finite Parameters

In our concept, we look for a boundary control θ_c, which has infinite degrees of freedom. The price we have to pay for this is high, because of the very complicated optimization system consisting of the forward and the adjoint system, which is hard to solve. Other concepts (for example Gunzburger et al., (2002) look for special control functions, which depend only of a few parameters. This restriction gives the possibility to minimize a given functional in the case of two parameters by a Newton method, and for one Newton iteration the forward problem must be solved three times.

Because of the more general concept a result, θ_c, of the presented optimization strategy will be optimal, in a more general sense, than prescribed temperature profiles, which depend only of one or two parameters. But the easier implementation of the method, given in Gunzburger et al. (2002), provides it to a valuable optimization tool.

5. Numerical Solution Method

The optimization system (11)-(16) and (26)-(34) is now under consideration for a numerical solution. The Navier-Stokes equation and the convective heat conduction equation are solved with a finite volume method; see Bärwolff (1994, 1997).

If we have cylinder-symmetric conditions, we can transform the adjoint equations into a cylindrical coordinate system. Using the adjoint divergence condition $div\,\mathbf{w} = 0$, we can write the adjoint equations in the following quasi-conservative form. We express the adjoint velocity $\mathbf{w}$ by

$$\mathbf{w} = (\mu, \nu, \omega)$$

in the cylindrical coordinate system with the radial component μ, the azimuthal component ν and the z-component ω and from (26) we get

$$\begin{gathered}-\mu_t - ((r\mu)_r/r)_r - \mu_{\varphi\varphi}/r^2 + 2\mu_\varphi/r^2 - \mu_{zz} + \mu u_r + \nu v_r + \omega w_r \\ -(ru\mu)_r/r - (v\mu)_\varphi/r - (w\mu)_z + v\nu/r + \xi_r = -(u - \bar{u}) - \kappa\theta_r\end{gathered} \tag{35}$$

$$\begin{gathered}\nu_t - ((r\nu)_r/r)_r - \nu_{\varphi\varphi}/r^2 - 2\nu_\varphi/r^2 - \nu_{zz} + \mu u_\varphi/r + \nu v_\varphi/r + \omega w_\varphi/r \\ +(\nu u - \mu v)/r - (ru\nu)_r/r + (v\nu)_\varphi/r - \nu\mu/r - (w\nu)_z - \xi_\varphi/r = -(v - \bar{v}) - \kappa\theta_\varphi/r\end{gathered} \tag{36}$$

$$\begin{gathered}-\omega_t - (r\omega_r)_r/r - \omega_{\varphi\varphi}/r^2 - \omega_{zz} + \mu u_z + \nu v_z + \omega w_z \\ -(ru\omega)_r/r - (v\omega)_\varphi/r - (w\omega)_z + \xi_z = -(w - \bar{w}) - \kappa\theta_z\end{gathered} \tag{37}$$

From equation (30), we get for the adjoint temperature κ as follows

$$-\kappa_t - \frac{1}{Pr}(r\kappa_r)_r/r - \frac{1}{Pr}\kappa_{\varphi\varphi}/r^2 - \kappa_{zz} - (ru\kappa)_r/r - (v\kappa)_\varphi/r - (w\kappa)_z = -\rho_\theta g w. \tag{38}$$

Equation (38) is a convective heat conduction equation and the discretization can be done as in Bärwolff (1997). In the equations (35)-(37), the terms

$$(\nabla\mathbf{u})^t\mathbf{w} \quad \text{and} \quad \kappa\nabla\theta$$

are not known from the classical Navier-Stokes equations. Using a staggered grid finite volume method, u and μ live at the same grid-points, also v and ν, w and ω, and θ and κ. For the first component of $(\nabla\mathbf{u})^t\mathbf{w}$ and $\kappa\nabla\theta$, we get, in a canonical way,

$$\begin{aligned}
&(\mu u_r + \nu v_r + \omega w_r)_{i+1/2jk} \approx \\
&\quad \mu_{i+1/2\,j\,k}\big[(u_{i+3/2\,j\,k} + u_{i+1/2\,j\,k}) - (u_{i+1/2\,j\,k} + u_{i-1/2\,j\,k})\big]/(2\Delta x_{i+1/2}) \\
&\quad +\nu_{i+1/2\,j\,k}\big[(v_{i+1\,j+1/2\,k} + v_{i+1\,j-1/2\,k}) - (v_{i\,j+1/2\,k} + v_{i\,j-1/2\,k})\big]/(2\Delta x_{i+1/2}) \\
&\quad + \omega_{i+1/2\,j\,k}\big[(w_{i+1\,j\,k+1/2} + w_{i+1\,j\,k-1/2}) - (w_{i\,j\,k+1/2} + w_{i\,j\,k-1/2})\big]/(2\Delta x_{i+1/2})
\end{aligned} \tag{39}$$

with

$$\nu_{i+1/2j\,k} = (\nu_{i\,j+1/2\,k} + \nu_{i+1\,j+1/2\,k} + \nu_{i\,j-1/2\,k} + \nu_{i+1\,j-1/2\,k})/4 \qquad \text{and}$$
$$\omega_{i+1/2\,j\,k} = (\omega_{i+1\,j\,k+1/2} + \omega_{i+1\,j\,k-1/2} + \omega_{i\,j\,k+1/2} + \omega_{i\,j\,k-1/2})/4,$$

and

$$\kappa\theta_r \approx 0.5(\kappa_{i+1\,j\,k} + \kappa_{ijk})\big[\theta_{i+1\,j\,k} - \theta_{ijk}\big]/\Delta x_{i+1/2}. \tag{40}$$

The solution of the discretized system (11)-(16) and (26)-(34) is difficult and expensive, because of the opposite time direction of the forward system (11)-(16) and the adjoint system (26)-(34). This means we know the forward solution $\mathbf{u}$, θ on the whole time interval $[0, T]$ to get the adjoint solution $\mathbf{w}$, κ and vice versa.

If we discretize the time interval $[0, T]$ by Z time-steps 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 following form are under consideration:

i) Choose a suitable start value of $\mathbf{u}$, θ.
ii) Solve the adjoint problem and get $[\mathbf{w}, \kappa, \theta_c](\mathbf{u}, \theta)$.
iii) Solve the forward problem and get $[\mathbf{u}, \theta](\theta_c)$.
iv) If not converged then go to ii).

In general such algorithm turn to be very expensive.

A realizable algorithm will be discussed in the next section.

6. Sub-optimal Control

The starting point for sub-optimal or instantaneous control is a time discretization of the Boussinesq equation system, i.e., in the case of an Euler backward time discretization with the time step parameter τ,

$$\mathbf{u} - \tau\Delta\mathbf{u} + \tau\nabla p = \tau\rho(\theta)\vec{g} - \tau(\mathbf{u}^o\cdot\nabla)\mathbf{u}^o + \mathbf{u}^o \quad \text{in} \quad \Omega, \tag{41}$$
$$-div\,\mathbf{u} = 0 \quad \text{in} \quad \Omega, \tag{42}$$
$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \Gamma, \tag{43}$$

where the upper index o means the values at the actual time level. Quantities without an index are considered at the new time level. The Euler backward time discretization of the heat conduction equation leads to

$$\theta - \tau \frac{1}{Pr} \Delta\theta + \tau(\mathbf{u}^o \cdot \nabla)\theta = \tau q^o + \theta^o \quad \text{in} \quad \Omega, \tag{44}$$

$$\theta = \theta_s \quad \text{on} \quad \Gamma_c, \tag{45}$$

$$\theta = 0 \quad \text{on} \quad \Gamma_{\mathrm{d}}, \tag{46}$$

Now, we look for a control θ_s, which minimizes the functional

$$J_s(\mathbf{u}, \theta_s) := \frac{1}{2}\int_{\Gamma_c} \theta_s^2 \, d\Gamma + \frac{1}{2}\int_{\Omega} |\mathbf{u} - \bar{\mathbf{u}}|^2 \, d\Omega. \tag{47}$$

For the solution of the boundary value problem (41)-(46) ${\bf u}$ for a control θ_s the functional $\hat{J}_s(\theta_s) := J_s(\mathbf{u}(\theta_s), \theta_s)$ will be minimal, thus, we have a stationary optimization problem per time step and with a sequence of such problems we will get a sub-optimal control θ_s over the time period $[0, T]$. The optimality system per time step is obtained following the same approach we used in the above discussed time-dependent case.

For the adjoint variables $\mathbf{w}$, ξ, κ and the control θ_s, we get the Lagrange function,

$$L(\mathbf{u}, p, \theta, \theta_s, \mathbf{w}, \xi, \kappa, \chi) = J_s(\mathbf{u}, \theta_s) + \langle \mathbf{w}, moment \rangle_\Omega - \langle \xi, div\, \mathbf{u} \rangle_\Omega + \langle \kappa, energy \rangle_\Omega + \langle \chi, \theta - \theta_s \rangle_{\Gamma_c}. \tag{48}$$

The necessary condition $\nabla L = \mathbf{0}$ gives the adjoint system,

$$\mathbf{w} - \tau\Delta\mathbf{w} + \nabla\xi = -(\mathbf{u} - \bar{\mathbf{u}}) \quad \text{in} \quad \Omega, \tag{49}$$

$$-\tau div\, \mathbf{w} = 0 \quad \text{in} \quad \Omega, \tag{50}$$

$$\mathbf{w} = 0 \quad \text{on} \quad \Gamma, \tag{51}$$

$$\kappa - \frac{\tau}{Pr}\Delta\kappa - \tau(\mathbf{u}^o \cdot \nabla)\kappa = -\tau\rho_\theta g\omega \quad \text{in} \quad \Omega, \tag{52}$$

$$\kappa = 0 \quad \text{on} \quad \Gamma, \tag{53}$$

$$\theta_s = \frac{\tau}{Pr}\frac{\partial\kappa}{\partial\mathbf{n}} \quad \text{on} \quad \Gamma_c. \tag{54}$$

The advantage of this technique is obvious, because we need to solve only a small stationary optimization problem. The results of Hinze (2001) showed the efficiency of the sub-optimal or instantaneous control strategy in the case of isotherm flows, and it could be shown that sub-optimal controls are very effective compared to optimal controls, i.e., the value of $\hat{J}(\theta_s)$ was only 10% higher than $\hat{J}(\theta_c)$ in the case of a boundary controlled backward facing step.

7. Conclusion

With the Lagrange parameter technique it is possible to derive an optimization system for a given functional, to provide an optimal control. The numerical solution of the fully time-dependent optimization system is not yet possible for realistic configurations.

Sub-optimal strategies with the used linearizations of (41) and (44) lead to a sequence of time-independent stationary optimization problems, which provide sub-optimal results near the optimal control. The developed strategies are now applied to the above discussed crystal melt problem in two and three dimensions.

Aknoledgements

The presented techniques and the resulting optimization systems are based on the results of a very close cooperation with Prof. Dr. Micheal Hinze, Koblenz/Hamburg, and the author thanks him very heartly.

References

[1] Bärwolff, G. and Hinze, M. (2006), Optimization of semiconductor melts, *ZAMM‐ Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik: Applied Mathematics and Mechanics*, 86(6), 423-437.
[2] Bärwolff, G., König, F. and Seifert, G. (1997), Thermal buoyancy convection in vertical zone melting configurations, *ZAMM‐Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 77(10), 757-766.
[3] Hinze, M. (2000), Optimal and instantaneous control of the instationary Navier-Stokes equations. habilitation thesis, Berlin, August 2000 (available on the webpage http:\\www.math.tu-dresden.de\~hinze).
[4] Hinze, M. (2001), Optimization of the Navier-Stokes equation, Adjoints workshop, Decin/Czech Republic, September 2001.
[5] Ladyzhenskaya, O. A. (1969), *The mathematical theory of viscous incompressible flow* (Vol. 2), New York: Gordon and Breach.
[6] Constantin, P., and Foias, C. (1988), *Navier-stokes equations*, University of Chicago Press.
[7] Gunzburger, M., Ozugurlu, E., Turner, J., and Zhang, H. (2002), Controlling transport phenomena in the Czochralski crystal growth process, *Journal of Crystal Growth*, 234(1), 47-62.
[8] Bärwolff, G. K. (1995), Numerical modelling of two-and three-dimensional external and internal unsteady incompressible flow problems, In *Computational fluid dynamics* (pp. 13-32), Springer, Berlin, Heidelberg.