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Optimization of a thermal coupled flow problem

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1. Introduction

During the growth of crystals crystal defects were 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 axisymmetric zone melting devices to an unsteady three-dimensional 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 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-interface decrease the crystal quality. Thus it makes sense to look 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

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

and problems with optimization functionals of the form

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

$\vec{u}$ is the velocity vector field in the melt and $\overline{\vec{u}}$ is the state, which we want to have, 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 and numerical solution method

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 the governing equations

$$u_t + (ruu)_r/r + (uv)_\varphi/r + (wu)_z - v^2/r = -p_r + \nabla\cdot(2\vec{S_r}) - 2S_{\varphi\varphi}/r\,, \tag{3}$$

$$v_t + (ruv)_r/r + (vv)_\varphi/r + (wv)_z + uv/r = -p_\varphi/r + \nabla\cdot(2\vec{S_\varphi}) + 2S_{r\varphi}/r\,, \tag{4}$$

$$w_t + (ruw)_r/r + (vw)_\varphi/r + (ww)_z = -p_z + \nabla\cdot(2\vec{S_z}) + Gr\,\theta\,, \tag{5}$$

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

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

in the cylindrical melt zone (height H, radius R). $\vec{S}$ denotes the stress tensor and u, v, w and p are the primitive variables of the velocity vector and the pressure, θ and c denote the dimensionless temperature and the Tellurite concentration.

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 inhomogeneous Dirichlet data, i.e. the melting point temperature. On the heated coat of the ampulla the experimentators gave us measured temperatures but we need Neumann conditions to describe the heating procedure physically correctly. The boundary conditions are of the form

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

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

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

The initial state was assumed as the neutral position of the crystal melt ($\vec{v} = 0$) 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

The use of formal Lagrange parameter technique with respect to the functional of type (1) leads in the case of the absence of solutal effects to the optimization system, which consists of the Navier-Stokes equations and the convective heat conduction equation and following a proposal of M. Hinze [2001], who is very successful in optimization of Navier-Stokes problems,

$$-\mu_t - \Delta\mu + (\nabla\vec{u})^t\mu - (\vec{u}\nabla)\mu + \nabla\xi == -(\vec{u} - \overline{\vec{u}}) - \kappa\nabla\theta \; on \; \Omega \times (0, T) \tag{11}$$

$$\mu = 0 \; on \; \Gamma \times (0, T), \; \mu(T) = 0 \tag{12}$$

$$-div\,\mu = 0 \; on \; \Omega \times (0, T) \tag{13}$$

$$-\kappa_t - \frac{1}{Pr}\Delta\kappa - \nabla\vec{u}\nabla\kappa = -Gr\,\mu \; on \; \Omega \times (0, T) \tag{14}$$

$$\kappa = 0 \; on \; \Gamma \times (0, T), \; \kappa(0) = 0 \tag{15}$$

$$-\theta_{c_{tt}} + \theta_c = \frac{1}{Pr}\partial_\eta\kappa = \chi \; on \; \Gamma_c \times (0.T) \tag{16}$$

$$\theta_{c_t}(0) = \theta_{c_t}(T) = 0\,, \tag{17}$$

where $\Omega \times (0, T)$ denotes the time cylinder of the problem and μ, ξ and κ are Lagrange parameters for the velocity, the pressure and the temperature.

4. Results

The optimization system (3)-(17) is now under consideration. The Navier-Stokes equation and the convective heat conduction equation are solved with a finite volume method (Bärwolff [1994, 1995, 1997]). The adjoint equations are also spatially discretized by a finite volume method. These investigations will going on and because of the computational amount (time and memory) we consider a two-dimensional simplification of the geometry. The results in progress will be presented on the conference.
Beside the complete optimization system (3)-(17) with the original forward problem and the adjoint backward problem a sub-optimal step by step strategy will be discussed.

5. References

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