Application of higher order BDF discretization of the Boussinesq equation and the convective heat conduction equation

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Motivation

During the growth of crystals there were observed crystal defects under some conditions of the growth device. As a result of experiments 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. 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.
For the investigation of this symmetry break a mathematical model of the crystal melt was formulated for

i) the theoretical description of the experimental observed behavior and

ii) the identification of critical parameters of the growth device, i.e. the evaluation of bifurcation points.

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. Heat conductivity and viscosity depend on the temperature.
For the velocity no slip boundary conditions are used. For the temperature we have at the interfaces between the solid material and the fluid crystal inhomogenous 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 physical correctly.
For the initial state we assume a 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.

Numerical solution method and mathematical aspects

A threedimensional finite volume code is used for the numerical solution of the above described non linear initial boundary value problem.
Because of the information loss about the heat fluxes over the boundary we have to solve an identification problem for finding suitable heat flux densities q for the formulation of the Neumann boundary condition of the form $-\lambda\frac{\partial\theta}{\partial n} = q$. q was identified in such a way, that the resulting temperature on the boundary is equal to a given measured value.
From mathematical point of view some bifurcation investigations are under consideration. But it's not possible to analyze the general nonlinear coupled problem described above. Simplifications with respect to the time dependency of the heat conductivity and the viscosity are necessary.
Quantitative bifurcation results of the general problem are only possible using numerical methods.
To get larger sized crystals it is nessecary to have a high resultion of the unsteady velocity and temperature field in space and time in crystal melt zones considering technologies to get larger sized crystals.
With respect to good possibilities of code parallelization expilicit backward finite differences (BDF) of higher order following [3] are used and discussed for the 3d numerical simulations of vertical zone melting and Czochralski techniques.

Results

A $(Bi_{1-x}Sb_x)_2Te_3$ crystal melt in an axisymmetric ampulla was investigated. We have the Prandtl number Pr, the Rayleigh number Ra and the aspect ratio α, i.e. height of the melt over the diameter of the ampulla, as parameters in the result of a dimension analysis.
With the numerical simulations using a threedimensional finite volume code developed by the author critical parameters of the crystal growth configuration and bifurcation points of the time behavior of the velocity and temperatur could be identified and the experimetal phenomena could be verified with

finding a critical value of $\alpha = \alpha_c = 1.45$. A theoretical mathematical bifurcation analysis gave some qualitative results.
Thus it was possible to define parameter intervals for a stable crystal growth configuration.
The following figures show the time history at two monitoring points of the melt and the frequency spectra for an over critical value of α, $\alpha = 3$, both from the experiment and the numerical simulation. The results show a very good agreement of the base frequency of the experiment and the simulation. The differences with respect to the amplitudes come from the fact, that the temperature can only be measured outside the ampulla, near the boundary.
The unsteady numerical results validate the theoretical analysis of [3] in the practical numerical simulation.

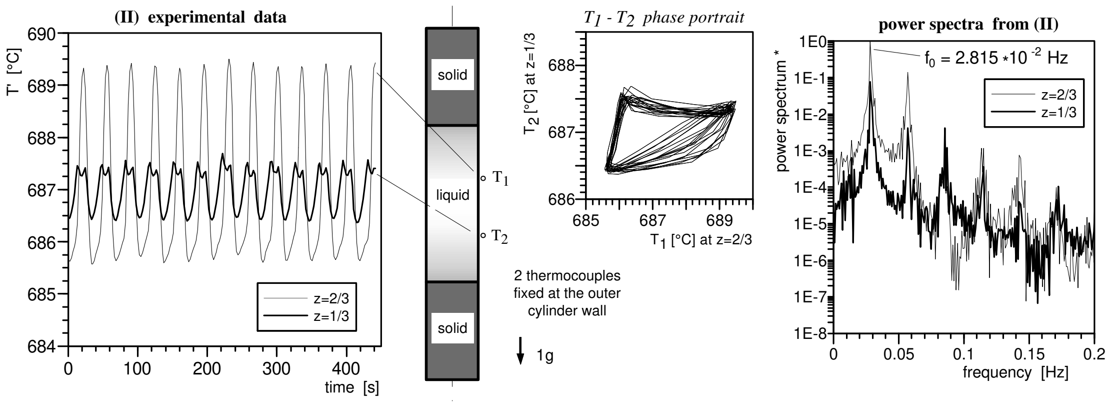

Figure 1: time history of the experiment

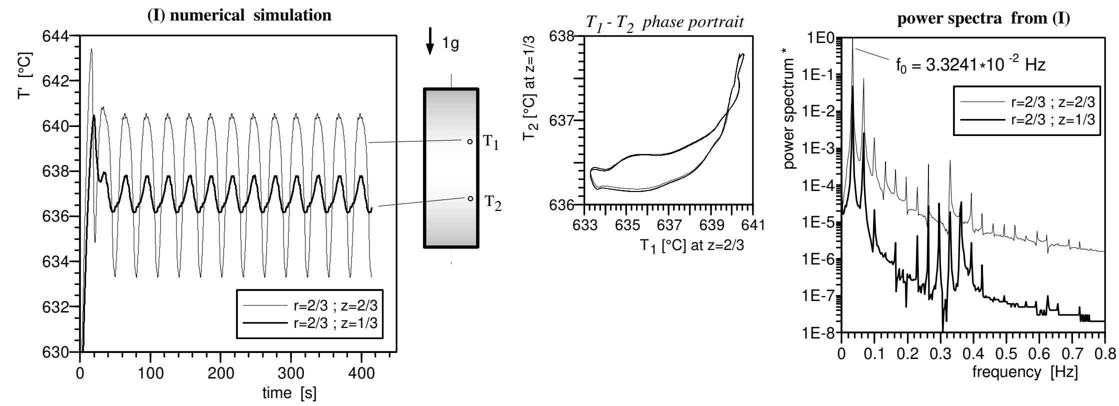

Figure 2: time history of the numerical simulation

References

[1] Bärwolff, G., König, F. and G. Seifert *Thermal buoyancy convection in vertical zone melting configurations, ZAMM 1997*

[2] König, F. and G. Bärwolff *Crystal growth of* $(Bi_{0.25}Sb_{0.75})_2Te_2$ *by zone melting technique under microgravity (IAF-Paper - 95 -J.1.02), 46th International Astronautical Congress, Oct. 2 - 6, Oslo, 1995*

[3] Emmrich, E. *Error Analysis for Second Order BDF Discretization of the Incompressible Navier-Stokes Problem, Proc. of the 4th Summer Conference on Numerical Modelling in Continuum Mechanics, Prague, August 2000*

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