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Three-dimensional stability calculations for hydrodynamic model of Czochralski growth

A.Yu. Gelfgat*

School of Mechanical Engineering, Faculty of Engineering, Tel-Aviv University, Tel-Aviv, Israel

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Abstract

Preliminary results obtained by a code aimed to the analysis of three-dimensional (3D) instability of axisymmetric melt flows in Czochralski crucible are described. The CPU time and the computer memory necessary for the comprehensive 3D stability analysis by a second-order finite volume method are estimated. Basing on a certain experimental configuration, we give an example of the stability diagram which shows how the critical temperature difference varies with the crystal rotation. We also show how critical temperature difference can be significantly increased by a weak rotation of the crucible and report corresponding stability diagrams.

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1. Introduction

The problem of melt flow instability in bulk crystal growth is well known since early experiments of Hurle [1]. Regarding the melt flow in a Czochralski crucible the first observations probably should be referred to Jones [2], who described a spoke pattern observed on the melt flow surface. Since then there were many experimental, theoretical and numerical studies that addressed instabilities in different crystal growth configurations. The vast majority of numerical studies on melt instabilities examine the time evolution of a two (2D)- or three-dimensional (3D) flow to make a conclusion of stability or instability of the studied flow developing in time. This approach has several disadvantages even in cases when only 2D flows are studied: the instability can be overlooked because of low tolerance of the numerical method; it is difficult to distinguish between numerical and physical instabilities; multiple flow states that depend on the initial conditions are usually missed. Accurate fully 3D computations do provide feasible results, however, are extremely CPU time consuming even when the most powerful computers are used. In many cases, computer restrictions do not allow one to perform accurate enough 3D computations. These restrictions can be partially removed in cases when the primary instabilities of initially axisymmetric flows are studied. Since a big part of bulk crystal growth setups is built to support axisymmetric conditions and considerable efforts are employed to keep the axisymmetric states stable, a problem of accurate computation of a primary instability as a function of governing parameters of the process necessarily appears. From a formal mathematical view point, this problem needs a calculation of an axisymmetric steady state of a process followed by the computation of the spectrum of the governing equations linearized in the vicinity of the steady state. To be realized numerically, this approach needs a fast solver for calculation of steady-state base flows and an effective eigensolver to approach the linear stability problem. This task seemed impossible for many years. However recently, due to a fast increase of available computer power and simultaneous development of numerical linear algebra algorithms this task becomes affordable.

The stability solver of this kind is being developed in our laboratory. It has been validated via a series of benchmark

*Tel.: +972 3 6407207; fax: +972 3 6407334.
E-mail address: gelfgat@eng.tau.ac.il.

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problems [3] and is applied now to a model corresponding to the melt flow in Czochralski crucibles. In the following, we describe a study of convergence of critical parameters with mesh refinement and give some estimations of CPU time and computer memory required for this kind of calculations. Then we report several examples of parametric stability studies based on the configuration of recently published experimental study [6].

2. Problem and numerical approach

We consider the same problem as the one defined in Ref. [4] and use the similar numerical method. The difference in the numerical approach is the implementation of a direct multifrontal sparse solver (we use MUMPs package) to calculate the LU decompositions of Jacobian matrices for both exact fully Jacobian Newton iteration and for the Arnoldi eigensolver. The details on this approach and convergence studies for some benchmark problems are given in Ref. [5]. The implementation of the multifrontal sparse solver significantly reduces the CPU time needed for solution of the stability problem, gives us a possibility to study the convergence of results with grid refinement and to perform parametric stability studies within the validated convergence.

For an illustrative study, we pick up one of the experimental configurations considered in Ref. [6] and study 3D instability of corresponding axisymmetric flows. We consider the flow of $NaNO_3$ melt with $Pr = 9.2$ in the crucible of the aspect ratio height/radius = 0.92 and the crystal-to-crucible radii ratio 0.5. The heating/cooling conditions are defined as

$$T = T_{\text{hot}} \text{ at the crucible sidewall;}$$
$$T = T_{\text{melting}} \text{ at the melt/crystal interface;} \quad (1)$$

$$T = T_{\text{hot}}\left(0.8571 + 0.1429\left(\frac{r}{R_{\text{crucible}}}\right)^2\right) \text{at the crucible bottom;} \quad (2)$$

$$\frac{\partial T}{\partial z} = -Bi(T - T_{\text{melting}}) \text{ at the free surface.} \quad (3)$$

Defining $\Delta T = T_{\text{hot}} - T_{\text{melting}}$ and using the data of Ref. [6] we estimate the Grashof and Marangoni numbers as $Gr = 1.9 \times 10^5 \Delta T$ and $Ma = 5400\Delta T$, where ΔT is

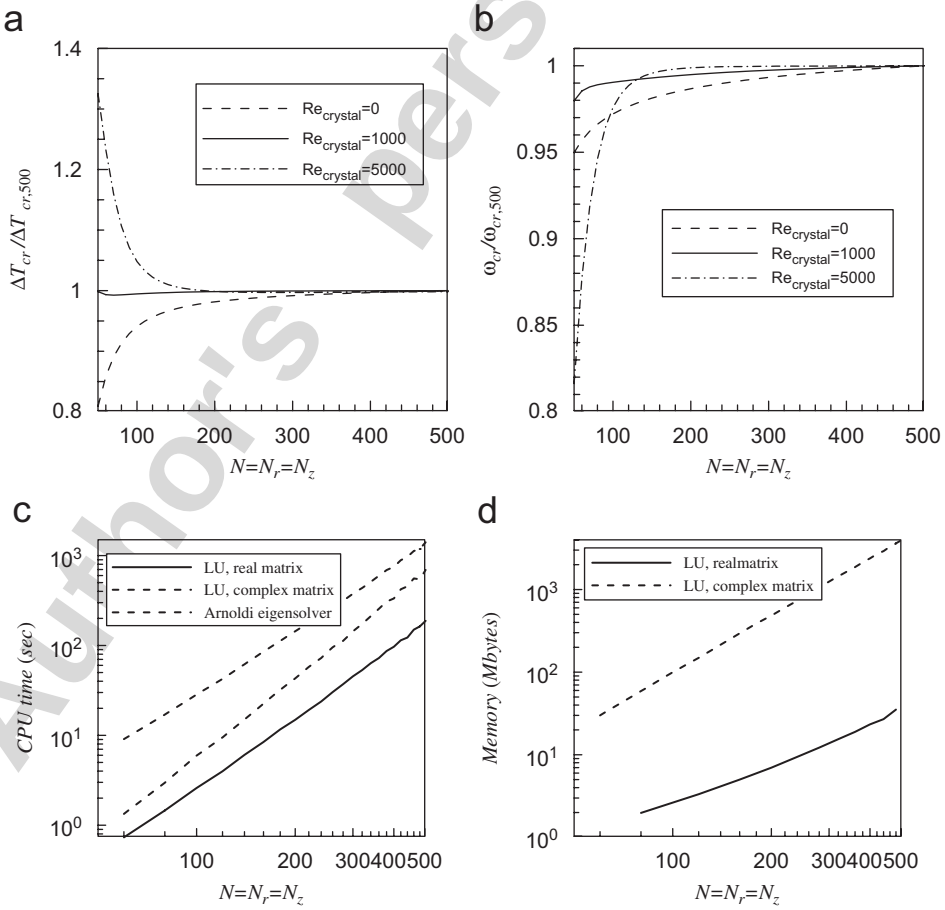

Fig. 1. Convergence of the critical temperature difference (a) and critical frequency (b) for the 3D instability of melt flow corresponding to the configuration of Ref. [6]. Frames (c) and (d) show the consumed CPU time and computer memory for the calculations reported in the frames (a) and (b). N = number of grid nodes in radial (N_r) and axial (N_z) direction.

measured in °C. The Biot number is fixed and estimated as $Bi = 0.1$. We also define two Reynolds numbers corresponding to the crystal and crucible rotation as $Re_{\text{crystal}} = \Omega_{\text{crystal}} R^2_{\text{crucible}}/\nu$ and $Re_{\text{crucible}} = \Omega_{\text{crucible}} R^2_{\text{crucible}}/\nu$, respectively.

Fig. 1a illustrates how the critical temperature difference corresponding to the onset of 3D instability converges with the mesh refinement. The uniform grids were used. We considered three cases corresponding to the stationary crucible. The crystal was either stationary ($Re_{\text{crystal}} = 0$) or rotating with a moderate ($Re_{\text{crystal}} = 1000$) or large ($Re_{\text{crystal}} = 5000$) angular velocity. At $Re_{\text{crystal}} = 0$ the instability sets in as a transition to an axisymmetric oscillatory state. At $Re_{\text{crystal}} = 1000$ and 5000 an azimuthal traveling wave with the azimuthal wavenumber $k = 1$ breaks the axial symmetry. In all cases the instability sets in with a characteristic critical frequency, whose convergence is illustrated in Fig. 1b. All the values in Fig. 1a and b are scaled by the value obtained on the finest grid of 500×500 nodes. It is emphasized that for a correct calculation of the critical parameters both the steady-state flow and the most unstable perturbation that breaks the axial symmetry must be calculated correctly. Therefore, the study of convergence of the critical parameters appears to be a demanding and representative exercise.

It follows from Fig. 1 that the fastest convergence of the critical values is observed for $Re_{\text{crystal}} = 1000$, for which the grid of 100^2 nodes yields a rather precise result. However, this is not a case for the stationary and rapidly rotating crystal. In these cases, the grids of order 300^2 or finer are needed to get an accurate result. This example shows that calculations of the 3D instability are rather demanding and cannot be performed on coarse grids. Apparently, the same requirements apply for the calculations of fully 3D supercritical states. Note that computations on coarse grids, which are rather often, can lead to qualitatively incorrect results. Theoretically, the mesh stretching can improve the convergence; however the results of Ref. [5], obtained for a set of benchmark problems, show that the choice of a good stretching is not so obvious. We also tried to use stretched grids for the present examples and found that beyond the grid size of approximately 200^2 the stretching does not yield a significant improvement.

Frames (c) and (d) of Fig. 1 show how the consumption of CPU time and the computer memory grows with mesh refinement. The calculations were performed on the Itanium-2 workstation. We report the time and the memory needed to calculate the LU decomposition of a real Jacobian matrix for the Newton iteration and a complex Jacobian matrix for the stability analysis. We also report a rather long time, which is consumed by the Arnoldi iterations after the corresponding LU decomposition is computed (Fig. 1c). It follows from Fig. 1c and d that the price for the use of the direct linear solver is the large memory consumed. Thus, the whole computational process on the grid consisting of 500^2 nodes needs more that 16 Gbyte computer memory. At the same time the basic block of these calculations, which consists of the solution for a steady state and an eigenproblem, consumes less than 1 h of CPU time. These data are for a single-processor calculation. Use of a multiprocessor computer will apparently reduce the CPU time, however can be more memory demanding.

3. Results

An example of the parametric stability analysis is given in Figs. 2 and 3. Using the azimuthal periodicity of the problem we decompose the 3D perturbation in Fourier series in the azimuthal direction. The linear stability problem separates for each Fourier mode $\sim\exp(ik\theta)$, which makes the azimuthal integer wavenumber k to be an additional governing parameter of the problem (for details see Ref. [4]). The first example corresponds to the flow with the stationary crucible. Fig. 2a shows the marginal temperature difference ΔT_k, which corresponds to the beginning of growth of the perturbations with $k = 0$, 1 and 2, versus the crystal Reynolds number. The largest value of

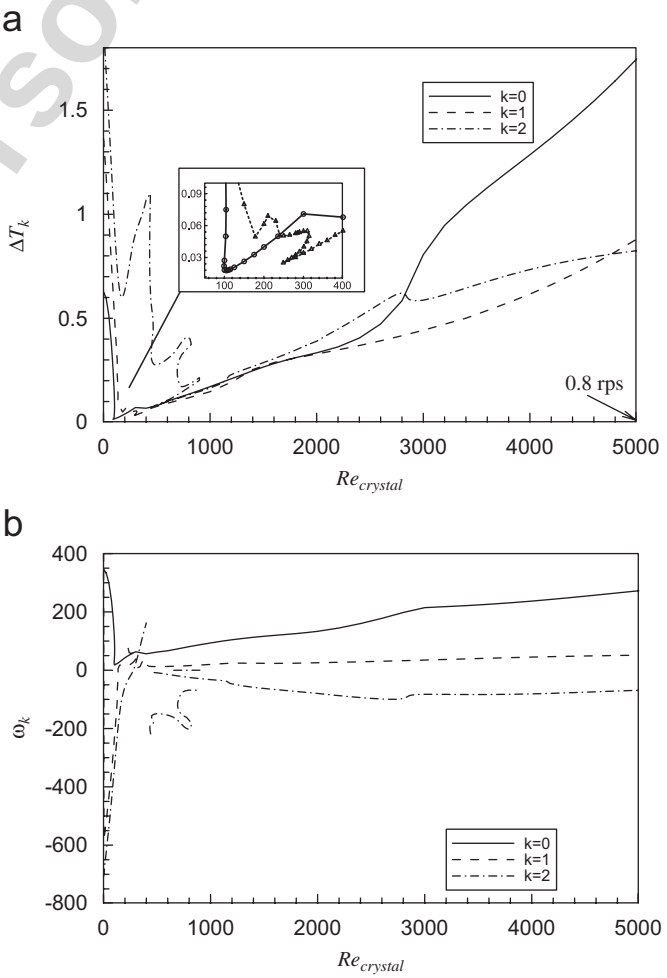

Fig. 2. Marginal temperature difference (a) and critical frequency (b) for the three-dimensional instability of flow configuration of Ref. [6]. $Re_{\text{crucible}} = 0$.

the crystal Reynolds number is 5000, which for the experimental data of Ref. [6] corresponds to the rotation frequency of approximately 0.8 rps. This rotation seems to be too fast for the Czochralski growth; however, for the melts with smaller viscosity or for the crucibles of larger radius the value of $Re_{\mathrm{crystal}} = 5000$ can be easily reached with a slower crystal rotation.

The critical value corresponds to the minimum of ΔT_k over all values of k. The values of ΔT_k for $k > 2$ always were above the values plotted in Fig. 2a. The marginal stability curves plotted in Fig. 2a show that with the increase of the crystal rotation the axisymmetric mode $k = 0$ and the 3D mode $k = 1$ yield the minimum of ΔT_k and several times replace each other as critical modes. For $Re_{\mathrm{crystal}} > 1000$ the mode $k = 2$ exhibit the marginal values of ΔT close to the critical ones. This means that in the supercritical regime the interaction of the two or even three modes can be expected, which will lead to rather complex non-linear dynamics.

Each azimuthal mode becomes unstable with a certain critical frequency, which is defined by the imaginary part of the leading eigenvalue (see Ref. [5] for details). The frequencies corresponding to the marginal stability curves of Fig. 2a are plotted in Fig. 2b. Note that the negative value of a frequency means that the unstable azimuthal traveling wave rotates in the direction opposite to the crystal rotation. It is seen from Fig. 2b that the frequencies corresponding to the different modes have different signs and magnitude, which also can make their interaction very complicated.

Fig. 3 illustrates a possibility of control of stability by means of a weak rotation of the crucible. We consider two fixed crucible Reynolds numbers 100 and -100, which for the data of Ref. [6] corresponds to the crucible rotation with the angular velocity of approximately 1 rpm. Positive and negative values of the Reynolds number correspond to the rotation in the same or opposite direction with respect to the crystal rotation. The flow is stable inside the neutral stability lines plotted in Fig. 3a and b and unstable outside them. Note that both stability diagrams have relatively narrow regions, where the critical temperature difference increases in several times or even in an order of magnitude compared with the stability limit corresponding to the stationary crucible. This rapid stabilization corresponds to the crystal Reynolds number of the order of 100, i.e., to the crystal rotation frequency of the order of 1 rpm, which is a practically reachable value. Fig. 4 shows that the patterns of meridional flow do not change significantly when the crucible rotates with $Re_{\mathrm{crucible}} = \pm 100$ or is stationary.

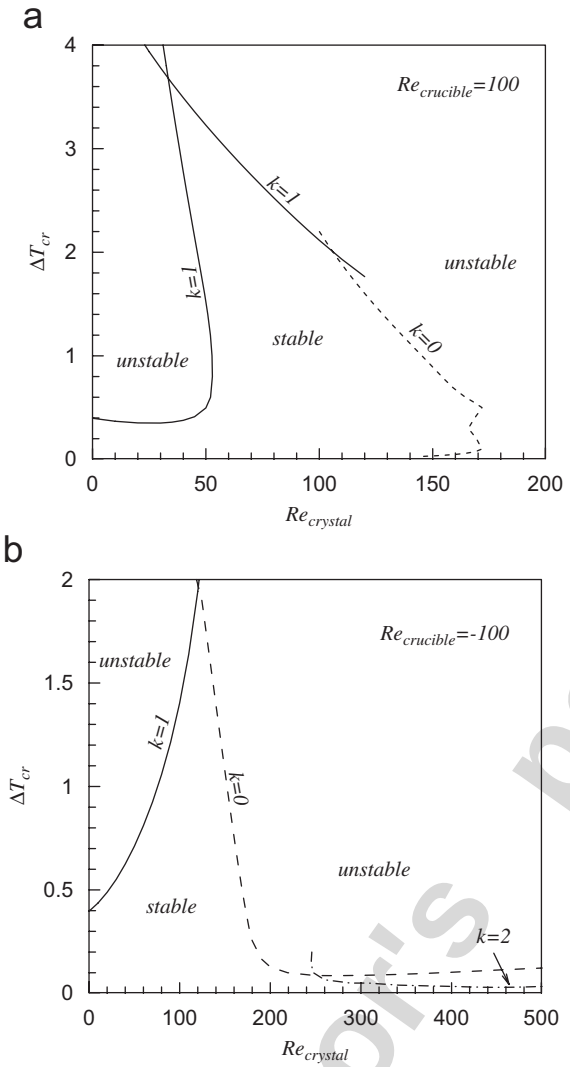

Fig. 3. Stability diagrams for the experimental configuration of Ref. [6] calculated for a slow crucible rotation.

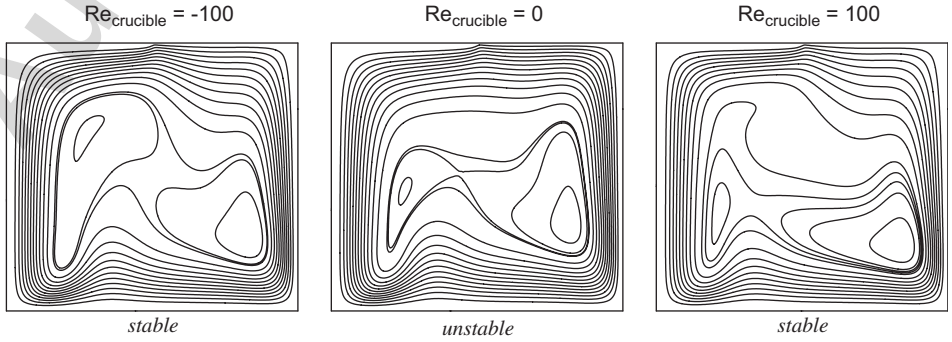

Fig. 4. Streamlines of meridional flow for $\Delta T = 1\,^{\circ}\mathrm{C}$, $Re_{\mathrm{crystal}} = 100$, and different rotations of the crucible.

At the same time, the stability properties of the flows illustrated in Fig. 4 change drastically (cf. Figs. 3 and 2a). To explain this it is necessary to analyze the change of the most unstable perturbations corresponding to all three flows, which cannot be done here due to the lack of space.

4. Concluding remarks

This study shows that the 3D stability analysis in Czochralski crystal growth configurations can be done in a realistic time on a rather moderate computer. The numerical approach can be easily extended to other bulk crystal growth configurations. An example for that can be found in Ref. [7]. It was concluded that to reach an acceptable accuracy for this kind of stability studies a rather good spatial resolution should be reached. For the second-order finite volume method used in the present study, we estimate that the grid must have about 100 grid nodes or more in the shortest spatial direction. This conclusion was made already in Ref. [5] where simpler benchmark problems were considered.

Similarly to Ref. [4] we gave an example of the stability diagram, which differs from one reported in Ref. [4] by the fact that the convergence of the numerical method was established before the calculations started. We also illustrated how stability of melt flow can be enhanced by a slow rotation of the crucible. Apparently, to find the mechanical or heating parameters, which stabilize the flow of a certain melt in certain conditions, the stability analysis should be repeated for each particular case.

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