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STABILITY AND INSTABILITY OF THERMOCAPILLARY CONVECTION IN MODELS OF THE FLOAT-ZONE CRYSTAL-GROWTH PROCESS

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I. Summary

The research performed under this project was concerned with the determination of conditions of guaranteed stability and instability for thermocapillary convection in a model of the float-zone crystal-growth process. This model, referred to as the *half-zone*, has been studied extensively, both experimentally and theoretically. Our own earlier research (Shen, Neitzel, Jankowski & Mittelmann (1990) determined, using energy-stability theory, sufficient conditions for stability to axisymmetric disturbances. Nearly all results computed were for the case of a liquid with Prandtl Number $Pr = 1$. Attempts to compute cases for higher Prandtl numbers to allow comparison with the experimental results of Preisser, Schwabe & Scharmann (1983) were unsuccessful, but indicated that the condition guaranteeing stability against axisymmetric disturbances would be a value of the Marangoni number Ma significantly *higher* than that at which oscillatory convection was observed experimentally. Thus, additional results were needed to round out the stability picture for this model problem.

The research performed under this grant consisted of the following: *i*) computation of energy-stability limits for non-axisymmetric disturbances; *ii*) computation of linear-stability limits for axisymmetric and non-axisymmetric disturbances; *iii*) numerical simulation of the basic state for half- and full-zones with a deformable free surface; and *iv*) incorporation of radiation heat transfer into a model energy-stability problem. Each of these is summarized briefly below.

A. Energy-stability results for a half-zone subjected to non-axisymmetric disturbances

Energy-stability theory provides sufficient conditions for stability against a specified class of finite-amplitude disturbances. The earlier research of Shen *et al.* (1990) considered axisymmetric disturbances only for two reasons: first, the size of the numerical problem for axisymmetric disturbances is significantly smaller than that for the 3-D case; second, if the results obtained for axisymmetric disturbances were an order of magnitude or more below the level of the experimental data, there would be little point in performing the more difficult computations for non-axisymmetric disturbances (since this could only result in a stability bound at the same Marangoni number or a *lower* one. Since these results indicated the 3-D computations may be valuable, they were done.

The numerical problem associated with the determination of these energy limits required the solution of a generalized eigenvalue problem with sparse, Hermitian, indefinite matrices. Since existing software was inadequate for these purposes, a new inverse-iteration algorithm was developed. This algorithm was successfully tested on the so-called "heated cylinder" problem to determine stability limits for the onset of convection in a circular cylinder heated from below (Mittelmann, Law, Jankowski & Neitzel 1992). Application of this algorithm to the half-zone problem yielded stability bounds which are in excellent agreement with Marangoni numbers at which the onset of oscillatory thermocapillary convection was observed in experiments of Velten, Schwabe & Scharmann (1991). These experiments were performed using potassium chloride (KCl) which has $Pr = 1$, alleviating the need to attempt calculations at higher Prandtl numbers. Although the azimuthal wave numbers which appear as the "most dangerous" from the theory do not agree with those measured by Velten *et al.* (1991) , there is no reason to suspect that they should, given the fact that energy theory provides a stability, rather than instability, bound.

B. Linear-stability results for a half-zone subjected to non-axisymmetric disturbances

Linear-stability theory, unlike energy theory, assumes that disturbance amplitude is infinitesimal in order to linearize the system of disturbance equations. Consequently, linear theory is capable of determining the conditions under which such small disturbances grow, at least initially, thereby providing a sufficient condition for instability. That is, a value of the Marangoni number Ma_L is obtained, such that disturbance growth is guaranteed for $Ma > Ma_L$. This result is complementary to that obtained from energy theory (Ma_E) and it can be demonstrated that $Ma_L \geq Ma_E$. Linear limits were computed for several of the same basic-state profiles considered for the energy-theory analyis.

The numerical problems associated with these computations were even more difficult to deal with. The linear theory equations do not yield a discretized set of equations which are Hermitian, like those of energy theory. Consequently, all non-zero elements of the matrices must be stored, rather than just those above the diagonal. The inverse-iteration algorithm employed so successfully for the energy theory calculations was modified again for these computations and, although convergence was quite slow, results were obtainable. The linear limits computed were reported in a recent paper by Neitzel, Chang, Jankowski & Mittelmann (1993) and are clearly above the level of both the energy limits and the experiments of Velten *et al.* In fact, if the level of the experimental data is accurate, it would appear that the instability is subcritical. Azimuthal wave numbers associated with the most dangerous modes correlate well with measured values.

C. Computation of steady thermocapillary flow with a deformable free-surface

Because all of the stability computations reported above were concerned with a basic state whose free surface was not permitted to deform, it was desirable to attempt basic-state computations which included this effect. These calculations were performed using the finite-element method with eight-noded rectangular elements for the velocity and temperature and four-noded elements for the pressure. The free-surface position was determined by assuming a shape, relaxing the normal-stress boundary condition to calculate the primitive field variables, then re-imposing the normal-stress condition to calculate a new free-surface shape. The process was repeated to convergence.

The results for a static zone (i.e., a half-zone for which the isothermal ends and surrounding environment were assumed to be at a uniform temperature) were compared to free-surface profiles measured in the laboratory of Professor Dietrich Schwabe. The agreement was nearly exact, lending credence to the numerical procedure. Results were also computed for thermocapillary convection in both terrestrial and microgravity environments. In all cases, the volume of liquid in the zone was assumed to be that which would correspond to a right circular cylinder. The free-surface deflections computed for microgravity deviated only slightly from this cylindrical shape; velocity profiles with and without gravity varied significantly (Hyer, Jankowski & Neitzel 1991).

D. Energy-stability computations with radiation heat transfer

All of the earlier stability work modeled the heat-transfer between the zone and its environment in terms of a simple convective mechanism. Since, crystal-growth processes operate at very high temperatures, radiation heat transfer effects are significant. It was desired, ultimately, to incorporate a radiation model into energy-stability computations for the half-zone, since it is this theory which would potentially provide a crystal grower with a boundary permitting the growth of striation-free material. The difficulty with doing this is that the radiation boundary condition is a nonlinear one which destroys the quadratic character of one of the functionals appearing in the energy theory. The result is a conditional stability limit which depends on the disturbance amplitude.

As a first attempt at this problem, it was decided to investigate the simplest basic state which would still allow the difficulties associated with radiation to be apparent. As a result, the problem of Rayleigh-Bénard convection between a pair of rigid, parallel planes was studied. The stability properties of this problem without radiation are well-known and linear-stability computations assuming the existence of radiation heat transfer have been computed (Christophorides & Davis 1970). For the energy analysis, the effect of radiation is always stabilizing. For this problem, it is possible to bound the non-quadratic parts of the troublesome functional by the quadratic part, so that the analysis may proceed in a standard fashion. For small disturbances, the energy-theory results are in agreement with those of Christophorides & Davis; for large values of the radiation parameter which appears, significant stabilization appears. The physical reasons for this are easily understood. The results will appear in a forthcoming paper (Bolander, Smith & Neitzel 1993).

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II. Papers and Presentations

Papers (refereed):

J. R. Hyer, D. F. Jankowski & G. P. Neitzel, "Thermocapillary Convection in a Model Float-Zone," AIAA Journal of Thermophysics and Heat Transfer, Vol. 5, pp. 577-582, 1991.

G.P. Neitzel, C. C. Law, D. F. Jankowski, & H. D. Mittelmann, "Energy Stability of Thermocapillary Convection in a Model of the Float-Zone, Crystal-Growth Process. Part 2, Non-Axisymmetric Disturbances," The Physics of Fluids A, Vol. 3, pp. 2841-2846, 1991.

H. D. Mittelmann, C. C. Law, D. F. Jankowski & G. P. Neitzel, "A Large, Sparse and Indefinite Generalized Eigenvalue Problem from Fluid Mechanics," SIAM Journal of Scientific and Statistical Computing, Vol. 13, pp. 411-424, 1992.

G. P. Neitzel, K.-T. Chang, D. F. Jankowski & H. D. Mittelmann, "Linear Stability of Thermocapillary Convection in a Model of the Float-Zone, Crystal-Growth Process," The Physics of Fluids A, Vol. 5, pp. 108-114, 1993.

H. D. Mittelmann, G. P. Neitzel, K.-T. Chang & D. F. Jankowski, "Iterative Solution of the Eigenvalue Problem in Hopf Bifurcation for the Boussinesq Equations," SIAM Journal of Scientific and Statistical Computing, to appear.

M. J. Bolander, M. K. Smith & G. P. Neitzel, "Thermal Instability with Radiation by the Method of Energy," in preparation.

Other papers:

H. D. Mittelmann, K.-T. Chang, D. F. Jankowski & G. P. Neitzel, "Stability of Thermocapillary Convection in Float-Zone Crystal Growth," in *Numerical Methods for Free Boundary Problems*, P. Neittaanmäki, ed., International Series of Numerical Mathematics, Vol. 99, pp. 58-69, 1991, Birkhäuser, Basel.

H. D. Mittelmann, K.-T. Chang, D. F. Jankowski & G. P. Neitzel, "Linear Stability of Axisymmetric Thermocapillary Convection in Crystal Growth," in Bifurcation and

Symmetry, E. Allgower, K. Böhmer, M. Golubitsky, eds., International Series of Numerical Mathematics, Vol. 104, pp. 275-284, 1992, Birkhauser, Basel.

Conference presentations:

G. P. Neitzel, K.-T. Chang, D. F. Jankowski & H. D. Mittelmann, "Linear Stability of Thermocapillary Convection in a Model Half-Zone," presented at the Forty-Fourth Meeting of the Division of Fluid Dynamics of the American Physical Society, Scottsdale, Arizona, November 1991.

G. P. Neitzel, K.-T. Chang, D. F. Jankowski & H. D. Mittelmann, "Linear Stability Theory of Thermocapillary Convection in a Model of Float-Zone Crystal Growth," presented at the Thirtieth AIAA Aerospace Sciences Meeting, Reno, Nevada, January 1992.

G. P. Neitzel, D. F. Jankowski, H. D. Mittelmann, Y. Shen, C. C. Law & K.-T. Chang, "Thermocapillary Convection Instability in Microgravity Crystal Growth," invited presentation at the VIIIth European Symposium on Materials and Fluid Sciences in Microgravity," Brussels, Belgium, April 1992.

H. D. Mittelmann, G. P. Neitzel, K.-T. Chang & D. F. Jankowski, "Iterative Solution of the Eigenvalue Problem in Hopf Bifurcation for the Boussinesq Equations," Proceedings of the Second Copper Mountain Conference on Iterative Methods, April 1992.

G. P. Neitzel, M. J. Bolander & M. K. Smith, "Thermal Instability by the Method of Energy," presented at the Forty-Fifth Meeting of the Division of Fluid Dynamics of the American Physical Society, Tallahassee, Florida, November, 1992.

R. J. Riley & G. P. Neitzel, "Linear Stability of Combined Thermocapillary-Buoyancy Convection in a Horizontal Slot," presented at the Forty-Fifth Meeting of the Division of Fluid Dynamics of the American Physical Society, Tallahassee, Florida, November, 1992.

H. D. Mittelmann, K.-T. Chang, D. F. Jankowski & G. P. Neitzel, "Hopf Bifurcation in Thermocapillary Convection Problems," presented at the conference on Theory and Numerical Methods for Initial-Boundary Value Problems, Oberwolfach, Germany, December, 1992.

H. D. Mittelmann, K.-T. Chang, D. F. Jankowski & G. P. Neitzel, "Linear Stability Analysis of the Boussinesq Equations," presented at the conference on Computational Methods for Nonlinear Phenomena, Oberwolfach, Germany, January, 1993.

Invited seminar presentations:

G. P. Neitzel

"The Fluid Dynamics of Materials Processing--An Example from Crystal Growth," presented at the College of Engineering, Tuskeegee University, Tuskeegee, Alabama, October 16, 1991.

"Stability of Thermocapillary Convection in a Model of the Float-Zone Crystal-Growth Process," presented at the Center for Microgravity and Materials Research, The University of Alabama in Huntsville, Huntsville, Alabama, October 29, 1991.

"Stability and Instability of Thermocapillary convection in a Model of the Float-Zone Crystal-Growth Process," presented at the Department of Chemical Engineering, Stanford University, Stanford, California, March 6, 1992.

"Stability and Instability of Thermocapillary convection in a Model of the Float-Zone Crystal-Growth Process," presented at the Microgravity Advanced Research Support (MARS) Center, Naples, Italy, October 9, 1992.

H. D. Mittelmann

"Stability of Thermocapillary Convection in Crystal Growth," Colloquium, University of British Columbia, Vancouver, Canada, October 7, 1991.

"Stability of Thermocapillary Convection--A Problem in Scientific Computing," Colloquium, University of Stuttgart, Stuttgart, Germany, April 21, 1992.

"Stability of Thermocapillary Convection--A Problem from Scientific Computing," Scientific Computing and Computational Mathematics Seminar," Stanford University, May 11, 1992.

"Stability of Thermocapillary Convection--A Problem from Scientific Computing," Colloquium, University of Tübingen, Tübingen, Germany, May 25, 1992.

"Computing Stability Bounds for Thermocapillary Convection," T-7 Seminar, Center for Nonlinear Studies, Los Alamos National Laboratory, June 9, 1992.

"Stability of Thermocapillary Convection--A Problem from Scientific Computing," Colloquium, Technical University of Dresden, Dresden, Germany, October 13, 1992.

"Stability of Thermocapillary Convection--A Problem from Scientific Computing," Colloquium, Technical University of Darmstadt, Darmstadt, Germany, January 11, 1993.

III. Student Degrees Received

At Arizona State University:

John R. Hyer, Master of Science, Spring, 1990

Kai-Ti Chang, Master of Science, Fall, 1991

Cindy C. Law, Master of Science, expected Summer, 1993

At The Georgia Institute of Technology:

Michael J. Bolander, Master of Science in Mechanical Engineering, Summer, 1992.