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Influence of liquid bridge volume on the onset of oscillation in floating-zone convection III. Three-dimensional model

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Abstract

An unsteady and three-dimensional model of the floating-half-zone convection on the ground is studied by the direct numerical simulation for the medium of 10 cSt silicon oil, and the influence of the liquid bridge volume on the critical applied temperature difference is especially discussed. The marginal curves for the onset of oscillation are separated into two branches related, respectively, to the slender liquid bridge and the fat liquid bridge. The oscillatory features of the floating-half-zone convection are also discussed. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Thermocapillary convection; 3D numerical simulation; Liquid bridge

1. Introduction

The floating-zone technique is one of the important methods for high-quality crystal growth, and has been applied to grow silicon and other semiconductor crystals. The floating-zone technique is performed successfully for grown crystal of larger diameter and is a favorable method in the space processing. Because of the limited opportunities of space experiments, most studies have been completed on the ground, and the liquid bridge of small typical scales is adopted to simulate

the thermocapillary convection, which dominates the process in the microgravity environment.

The thermocapillary oscillatory convections in the floating-half-zone were observed for the first time in 1978 [1,2]. Because of the pressure gradient in the direction of the earth's gravity, the configuration of the liquid bridge cannot be cylindrical, but is usually a shape of calabash. Many theoretical analyses assume a simplified model, in which the liquid bridge is a cylinder. The different volumes of the liquid bridge relate to different shapes. The critical condition for the onset of oscillation in a cylindrical liquid bridge of the floating-zone convection may be different from the one in a calabash liquid bridge; and also the situation in a slender liquid bridge may be different from that in a fat liquid bridge. The conclusions of both the experimental and the theoretical studies show that

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the volume of the liquid bridge is another critical geometrical parameter, which is more sensitive and complex than the geometrical aspect ratio.

The ground-based experiments show that, the critical Marangoni numbers or the critical applied temperature differences depend on the volumes of the liquid bridge [3–6]. The systematic studies of the ground-based experiments discovered that the marginal curves for the onset of oscillation have two branches, which associate, respectively, with the slender liquid bridge and the fat liquid bridge; and a gap region with higher critical values is there between the two branches. The results were published as paper I [7]. The numerical simulation was studied as the first step, by a simplified two-dimensional model, and the numerical conclusion agrees qualitatively with the experimental conclusion as shown in paper II [8]. However, a more reasonable model of the onset oscillation in the liquid bridge of a floating-half-zone convection needs to be three-dimensional. Recently, several numerical simulations for three-dimensional oscillatory thermocapillary convection were reported [9,10], and the unsteady and three-dimensional model for studying the effect of volume ratio is studied in the present paper as paper III.

The evolutionary process of the floating-half-zone convection is studied by the numerical simulation method in a small liquid bridge, and the convection is responded to the increase of the applied temperature difference. There is no convection at the beginning when the applied temperature difference is zero, and the steady convection transfers to the oscillatory convection if the applied temperature difference is increased over its critical value. The numerical model is discussed in the next section, and the onset of oscillatory oscillation is analyzed in Section 3. The dependence of liquid bridge volume on the critical applied temperature difference is given in Section 4, and the last section is the conclusion. The results of the three-dimensional model are more reasonable than those of the two-dimensional ones.

2. Model of numerical simulation

For comparison with the experiments, the 10 cSt silicon oil is used as the liquid medium in a usual

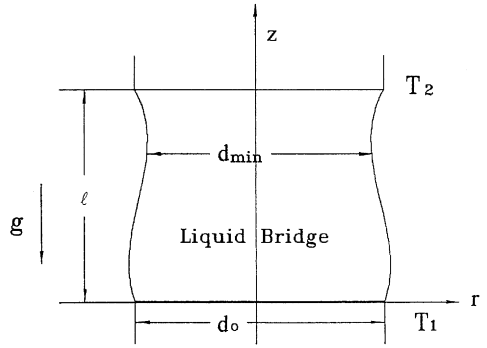


Fig. 1. The schematic diagram of the liquid bridge.

model of floating-half-zone with a height l of 4 mm. Two co-axial copper rods have same diameters d_0 of 5 mm. The temperature T_1 at the lower rod is kept constant during the process, and the temperature T_2 at the upper rod is heated at a rate of 4°C/s , i.e. $T_2 = T_1 + (4^\circ\text{C/s})t$, where t is the time. The shape of the free surface depends on the volume of the liquid bridge as shown in Fig. 1, which is the static configuration of the liquid bridge and is considered as unchangeable during the calculating process. A cylindrical coordinate system (r, θ, z) is adopted, and the center of the lower rod is taken as the origin of the coordinate system.

The nondimensional quantities are defined as follows:

$$\xi = \frac{r}{\ell}, \quad \zeta = \frac{z}{\ell}, \quad \tau = \frac{t}{\ell/v_*}, \quad (1)$$

$$U = \frac{u}{v_*}, \quad V = \frac{v}{v_*}, \quad W = \frac{w}{v_*}, \quad \Theta = \frac{T}{T_* - T_1}, \quad (2)$$

where T_* is a referential temperature and T_* is 45°C in the present calculation. (u, v, w) is the velocity vector in the cylindrical coordinate system, the typical velocity $v_* = -|\partial\sigma/\partial T|(T_* - T_1)/\rho\nu$ and σ, ν, ρ are, respectively, the surface tension, kinematic viscosity, density of the liquid. The following typical parameters are important in the process:

$$\text{Ma} = \frac{v_*\ell}{\kappa}, \quad \text{Re} = \frac{v_*\ell}{\nu}, \quad \text{Gr} = \frac{g\beta(T_2 - T_1)\ell^3}{\nu^2}, \quad (3)$$

$$\text{B}_d = \frac{\rho g \beta \ell^2}{|\partial\sigma/\partial T|},$$

where κ and β are, respectively, the thermal diffusion coefficient and the expansion coefficient. The parameters in Eq. (3) are named, respectively, the Marangoni number, the Reynolds number, the Grashof number and the dynamic Bond number. The Prandtl number may be obtained by $\text{Pr} = \text{Ma}/\text{Re}$. In addition, there are two typical geometrical parameters, that is, the geometrical aspect ratio $A = l/d_0$ and the ratio of the liquid bridge volume V to the cylindrical volume V_0 . The dynamic bond number B_d describes the relative importance of the effect of the gravity and the effect of the surface tension, and is $O(10^\circ)$ in order of magnitude in case of the present paper. This means that the thermocapillary effect is comparable with the gravitational effect.

Introducing the stream function vector $\Psi = (\psi_\xi, \psi_\theta, \psi_\zeta)$ and vorticity vector as $\Omega = (\Omega_\xi, \Omega_\theta, \Omega_\zeta)$ as

$$\nabla \times \Psi = \mathbf{V}, \quad \nabla \times \mathbf{V} = \Omega. \quad (4)$$

The basic equations are then, written as follows:

$$\nabla \times \nabla \Psi = \Omega \quad (5)$$

$$\text{Re} \left[\frac{\partial \Omega}{\partial \tau} + (\mathbf{V} \cdot \nabla) \Omega - (\Omega \cdot \nabla) \mathbf{V} \right] = \nabla^2 \Omega + \text{Re} \nabla \times \mathbf{F}, \quad (6)$$

$$\text{Ma} \left[\frac{\partial \Theta}{\partial \tau} + (\mathbf{V} \cdot \nabla) \Theta \right] = \nabla^2 \Theta, \quad (7)$$

where the nondimensional body force \mathbf{F} is the gravity $g\ell/v_*^2$.

The boundary conditions at the solid–liquid interface are

$$\Theta(\tau, \xi, \theta, 0) = 0, \quad \Theta(\tau, \xi, \theta, 1) = f(\tau), \quad (8)$$

$$\psi_\xi = 0, \quad \psi_\theta = 0, \quad \partial \psi_\zeta / \partial \zeta = 0, \quad (\zeta = 0, 1) \quad (9)$$

$$\Omega_\xi = -\partial V / \partial \zeta, \quad \Omega_\theta = \partial U / \partial \zeta, \quad \Omega_\zeta = 0, \quad (\zeta = 0, 1) \quad (10)$$

where

$$f(\tau) = \begin{cases} \alpha_T \tau \ell / (\Delta T^* V_*), & t < \Delta T / \alpha_T, \\ 1, & t \geq \Delta T / \alpha_T. \end{cases}$$

The boundary conditions at the free surface $\xi = R(\zeta)$ are as follows:

$$\psi_s = 0, \quad \psi_\theta = 0, \quad \nabla \cdot \Psi = 0, \quad (11)$$

$$\partial \Theta / \partial n = 0, \quad (12)$$

$$\Omega_\xi = \frac{1}{\xi} \frac{\partial W}{\partial \theta} - \frac{\partial V}{\partial \zeta}, \quad (13)$$

$$\Omega_\theta = \left[\frac{1 + R'^2}{1 - R'^2} \frac{\partial \Theta}{\partial s} + \frac{2R'}{1 - R'^2} \left(\frac{\partial U}{\partial \xi} - \frac{\partial W}{\partial \zeta} \right) + \frac{\partial U}{\partial \zeta} \right], \quad (14)$$

$$\Omega_\zeta = \frac{\sqrt{1 + R'^2}}{R} \frac{\partial \Theta}{\partial \theta} + 2 \frac{\partial V}{\partial \xi} - R' \left(\Omega_\xi + 2 \frac{\partial V}{\partial \zeta} \right), \quad (15)$$

where the free surface is described as $\xi = R(\zeta)$, and s denotes the surface coordinate perpendicular to the θ direction on the free surface. It should be noted that, the applied temperature difference $\Delta T = T_* - T_1$ in the unsteady model of the present paper is increased with a heating rate of 4°C/s from 0.01 to 45°C . When $\Delta T > 45^\circ\text{C}$ the applied temperature difference will maintain at 45°C .

The finite element method and characteristic line method are jointly used, respectively, to the diffusion terms and convection terms in the numerical simulation. The volume of the liquid bridge is divided into 10 758 volume elements with 2064 nodes. The detailed method of the calculations is discussed in Ref. [11].

3. The onset of oscillation

The transition of the velocity fields in the floating-half-zone convection is observed experimentally by the PIV method for a transparent liquid bridge, and the flow pattern changes from the axial symmetrical and steady cell to the axial asymmetrical and oscillatory cell in a vertical cross-section of a liquid bridge. Recently, the flow pattern in a horizontal cross-section was also observed, and the results show fruitful and complex

structures in comparison with the pattern in the vertical cross-section [12]. All the components of fluctuation velocity fields have the same order of magnitude of the total velocity, and show a strong nonlinear behavior. This nonlinear behavior given by the experiments is important characteristics of the transient process in the floating-half-zone convection and cannot be analyzed by the linear instability analysis.

The most conspicuous feature of the onset of oscillation in a three-dimensional model is the azimuthal velocity, which is observed in the experiments [12] but cannot be described in a two-dimensional model. The evolution processes for both azimuthal velocity and temperature in a slender liquid bridge with a volume ratio $V/V_0 = 0.58$ are given in Fig. 2 at four locations each with 90° of phase difference in a cross-section $\zeta = 0.55$ on the free surface. It could be seen that the azimuthal velocity transits from zero to the oscillatory profiles if the applied temperature difference increases and is larger than a critical value. The oscillatory component of the azimuthal velocity is larger, and the average component of azimuthal velocity is nearly zero. The results also show that the frequency of oscillatory azimuthal velocity is the same as that of the temperature.

To describe the detailed features of the deviation from this steady and axisymmetric convection, the two quantities may be defined, respectively, for azimuthal velocity and temperature as follows:

$$\delta_v = \frac{V_{\max} - V_{\min}}{V_m}, \quad \delta_T = \frac{T_{\max} - T_{\min}}{\Delta T}, \quad (16)$$

where V_{\max} and V_{\min} are, respectively, the maximum and minimum azimuthal velocity in a vertical cross-section $\zeta = 0.55$, V_m is the maximum velocities in the liquid bridge, T_{\max} and T_{\min} are, respectively, the maximum and minimum temperatures in $\zeta = 0.55$. Fig. 3 gives the evolution of the oscillatory quantities for a slender liquid bridge $V/V_0 = 0.58$, and the oscillatory quantities $\delta_v = O(1)$ and $\delta_T = O(10^{-1})$. These results mean that the oscillatory component of the azimuthal velocity has the same order of magnitude as the maximum velocity but the oscillatory temperature

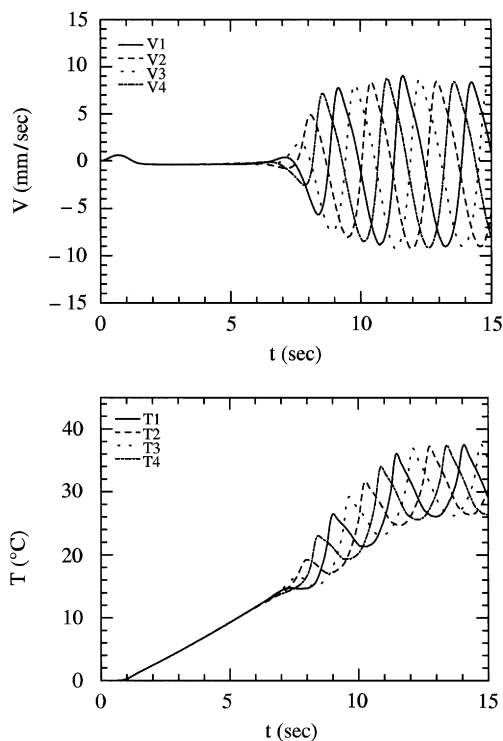


Fig. 2. The evolution processes of azimuthal velocity (upper) and temperature (lower) at four spots ($\varphi = 0, \pi/2, \pi, 3\pi/4$) of the boundary in the cross-section $\zeta = 0.55$.

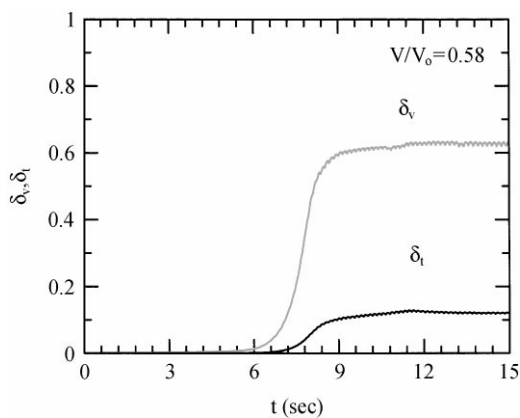


Fig. 3. The evolution processes of oscillatory quantities δ_v and δ_T .

is smaller by one order of magnitude than the average temperature. Similar conclusions are obtained for the fat liquid bridge.

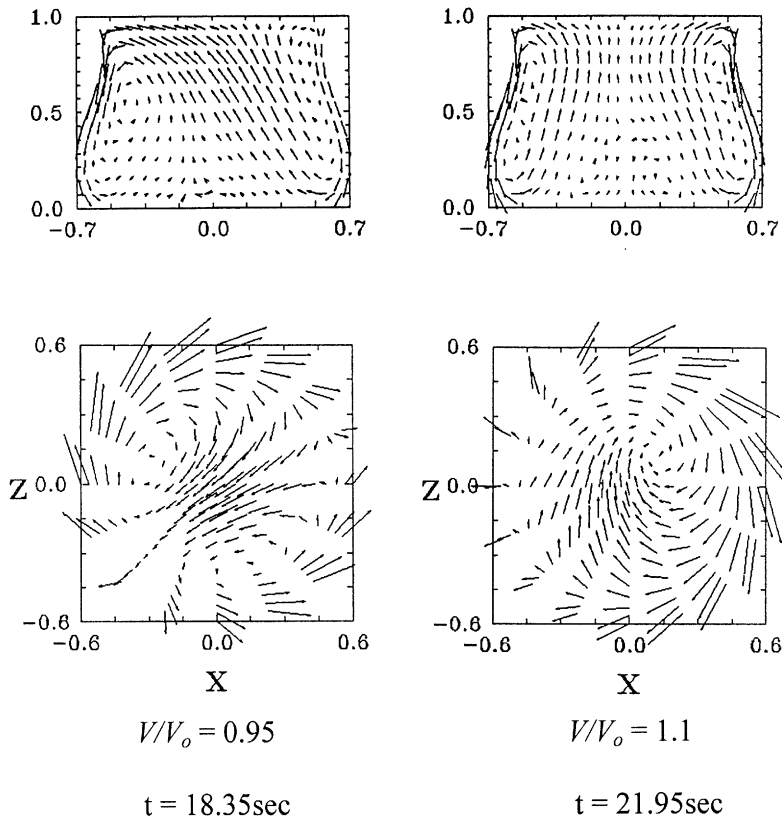


Fig. 4. The flow patterns at the vertical cross-section (upper) and the horizontal cross-section (lower).

The velocity fields in a liquid bridge of a complete developed oscillatory convection are given in Fig. 4. The upper parts and lower parts relate, respectively, to the vertical cross-section $\theta = 0, \pi$ and the horizontal cross-section $\zeta = 0.55$, and the left parts and the right parts relate, respectively, to the slender liquid bridge $V/V_0 = 0.95$ at moment $t = 18.35$ s and fat liquid bridge $V/V_0 = 1.1$ at moment $t = 21.95$ s. The isotherms in the horizontal cross-section for a slender liquid bridge $V/V_0 = 0.95$ and a fat one $V/V_0 = 1.1$ are shown in Fig. 5, from which it is obvious that the patterns rotate with time. The velocity and temperature distributions are relatively more axially asymmetric in case of a fatter liquid bridge than in case of a slender liquid bridge, and the temperature profiles show an instability with azimuthal mode $m = 1$ for both a slender liquid bridge and a fat liquid bridge.

4. The influence of liquid bridge volume

The onset of both temperature and velocity oscillations in the liquid bridge of the floating zone convection may be seen clearly in Figs. 2 and 3. However, the onset oscillation of the azimuthal velocity strongly shows the nonlinear feature, and may be selected as a better critical quantity to judge the onset process. The small deviation from the basic steady and axisymmetric state is defined as the moment of onset of oscillation in the linear stability analysis. In the nonlinear theory of the present paper, the deviation from the steady and axisymmetric convection in a floating-half-zone may be defined by the criterion of $\delta_v/2 = 0.01$ for the case of a given ratio of volume as shown in Fig. 3. Then, the critical applied temperature difference or the critical Marangoni number depending

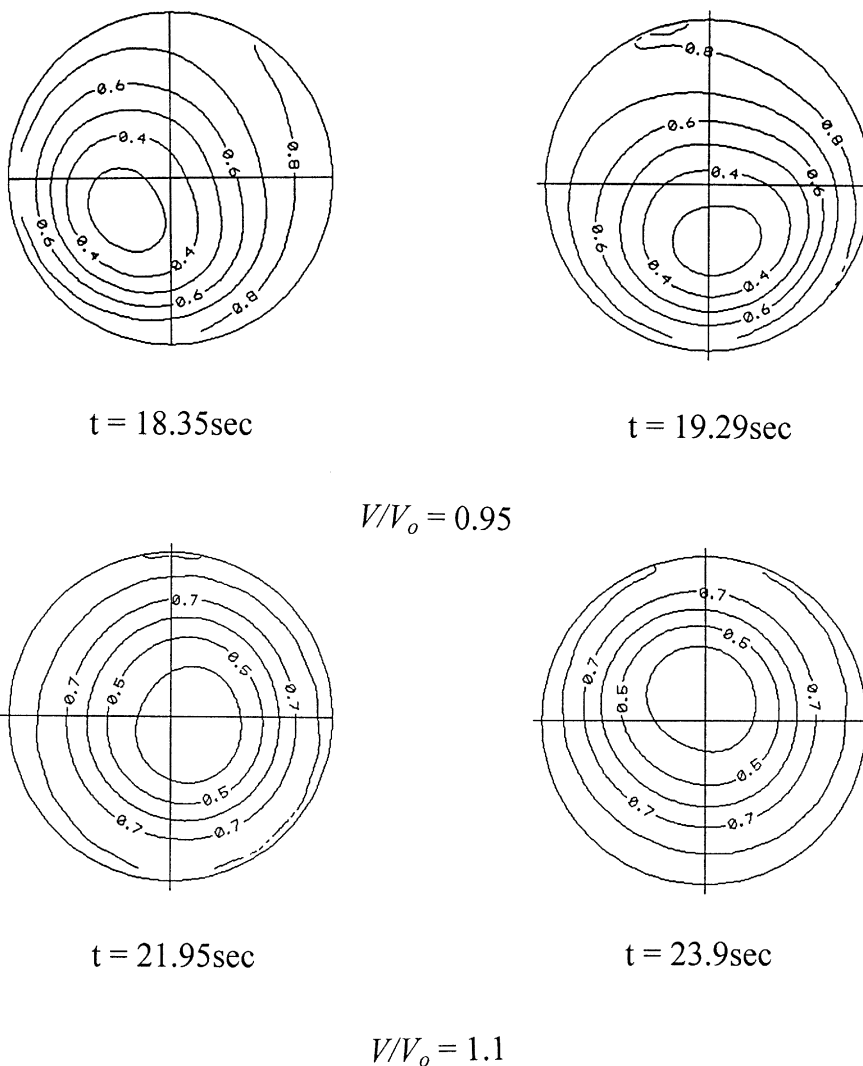


Fig. 5. The isotherms at the the horizontal cross-section.

on the ratio of volume, may be obtained in every case for different ratio of volume of liquid bridge. The calculated results are summarized in Fig. 6a.

The results of the unsteady and three-dimensional numerical simulation shows that, the marginal instability curve has two branches, associated with the slender liquid bridge and fat liquid bridge, respectively. There is a small gap in region $0.95 < V/V_0 < 0.97$, which separates the two branches. The flow features and temperature distributions are quite different in the two branches as

discussed in the last section. The marginal instability curve in case of Fig. 6a relates to the transition from the steady and axisymmetric convection to the oscillatory convection for the slender branch but to the steady asymmetric convection for the fat branch. The results show that, there are two bifurcations in case of small geometrical aspect ratio, and for the fat liquid bridge, the steady and axisymmetric convection transits firstly to the steady and axial asymmetric convection, then to the oscillatory convection in the liquid bridge of large Prandtl

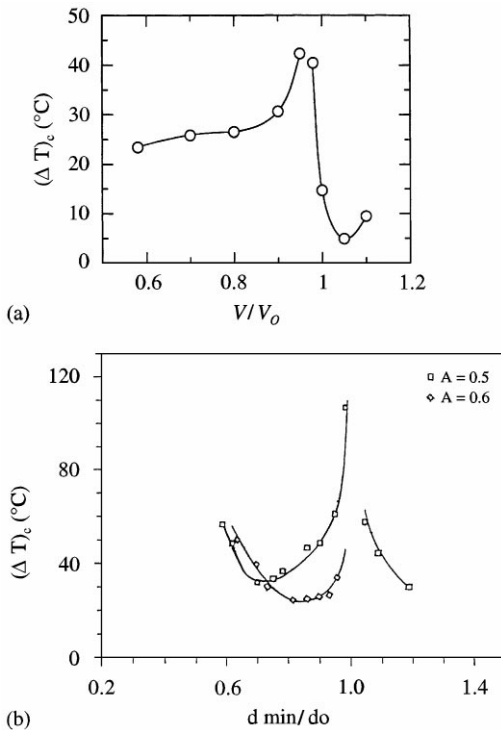


Fig. 6. The dependence of critical applied temperature on the ratio volume: (a) the results from the present numerical simulation; (b) the experimental results.

number. The details of this feature will be discussed elsewhere.

The dependencies of critical applied temperature differences on the ratio volumes were obtained experimentally for the liquid bridges, which were 5.5 mm in diameter with an aspect ratio $A = 0.6$ and 0.5, respectively, and filled with 10 cSt silicon oil. The marginal curves for the onset of oscillation calculated by using three-dimensional model agree with the experimental results as shown in Fig. 6b.

5. Discussions

The unsteady and three-dimensional model is applied to study the onset of oscillation in a floating-half-zone convection, especially the dependence of critical Marangoni on the volume of liquid bridge. The general conclusions of the three-dimen-

sional model agrees with those of the two-dimensional model, but the three-dimensional model is more reasonable in comparison with the two-dimensional model. The three-dimensional model gives the process of the onset oscillation, where the fluctuation velocity and the total velocity have the same order of magnitude and the fluctuation temperature is one order of magnitude smaller than the average temperature. These conclusions agree with the experiments, and are better than the ones obtained using the two-dimensional model.

From the view point of fluid mechanics it is easy to expect that the volume of liquid bridge is a critical parameter for the onset of oscillation. The instability analysis of isothermally liquid bridge showed the dependence of liquid bridge volume and gave the stability region for the liquid bridge depending on its volume [13]. In the case of the instability analysis of the thermocapillary convection in a floating-half-zone, the perturbed kinetic energy E_{kin} equals the addition of the viscous dissipation — D , the work M done by the thermocapillary force on the free surface and the interactive term I_r of perturbed velocity and basic velocity (see, for example Ref. [14]).

$$\frac{\partial E_{kin}}{\partial t} = -D + M + I_v. \quad (17)$$

The work M depends sensitively on the configuration of liquid bridge, which relates to the volume of liquid bridge.

The evolution of the azimuthal velocity is discussed in the three-dimensional model, and it describes one of the features on the strong nonlinear behavior of the transition from steady convection to oscillatory convection. This nonlinear feature may discover different behavior described by the linear theory. In the present paper, a criterion based on the azimuthal velocity is defined for the deviation from the steady and axisymmetric convection in the floating-half-zone convection, and this criterion may be reasonable, especially for the numerical simulation.

The conclusion of the three-dimensional model confirm in general that, the volume of the liquid bridge is a sensitive critical parameter for the onset of oscillation, and the marginal curves of the onset

oscillation is divided into two branches related, respectively, to the slender liquid bridge and the fat liquid bridge. These conclusions agree with those of two-dimensional model. The gap region is very narrow and the marginal curves are relatively smooth in the three-dimensional model than in the two-dimensional model. The three-dimensional model gives the evolution of three velocity components including the azimuthal velocity, and this advantage is important in understanding of the nonlinear features of the transient process in the floating-half-zone convection.

In the present paper, the transient process is studied in the typical case of a liquid bridge of 10 cSt silicon oil with a fixed geometrical aspect ratio $A = 0.8$, and the main features of the onset oscillation process are analyzed by using the three-dimensional model. The studies of broader parameter ranges will be beneficial in the understanding of the process, and needs to be performed in the future.

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