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Thermocapillary convection in a differentially heated two-layer annular system with and without rotation

Han-Ming Li, Wan-Yuan Shi *

Key Laboratory of Low-grade Energy Utilization Technologies and Systems of Ministry of Education, College of Power Engineering, Chongqing University, Chongqing 400044, China

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ABSTRACT

Thermocapillary convection in a differentially heated bilayer annular pool consisting of 5cS silicone oil and HT-70 is investigated by a series of three-dimensional numerical simulations. Both systems with and without rotation are considered. The results indicate that the thermocapillary convection is steady and axisymmetric when the Marangoni number is small. The system rotation suppresses the radial flow in the lower layer. Once the Marangoni number exceeds a threshold value, three-dimensional oscillatory flow occurs in both layers simultaneously. The stability diagram reveals that weak rotation destabilizes the axisymmetric flow, while stronger rotation retards the onset of oscillatory flow. The wave patterns for oscillatory flow appear in the form of blade-like waves propagating outward. The surface oscillation and the interface oscillation always share a common frequency but have about a half-period phase lag. In the rotating pool, single group of curved hydrothermal waves propagates in the azimuthal direction opposite to the pool rotation. As the rotation rate increases, the wave number increases while the oscillation frequency decreases.

1. Introduction

Thermal convection in two-layer system is a common phenomenon that is of great importance in various processes such as earth mantle convection [1] and single crystal growth [2]. In the process of single-crystal growth from the melt containing some volatile components (such as GaAs, PbTe), the evaporation of more volatile component may lead to an inhomogeneous change of composition and further reduce quality of the grown crystal. In order to prevent evaporation, liquid encapsulation technique, such as Liquid Encapsulated Czochralski (LEC) method [3], was developed. In this technology, a suitable liquid encapsulant covers the melt surface to prevent evaporation. Meanwhile, the encapsulant unavoidably introduces a liquid–liquid interface tension between the encapsulant and the melt. Due to the existence of a horizontal temperature gradient in the crucible in a LEC system, thermocapillary convections are generated, driven by the tension gradients on both the encapsulant's surface and the encapsulant-melt interface. Physically, it is referred to as the thermocapillary convections in two-layer system in literature [4]. If such a thermocapillary convection is coupled with the crucible rotation, which is a common approach to smoothen the non-uniform heating from the heaters in LEC furnace, the convection would become quite complex and influence the flow instability.

Over the past few decades, numerous experimental works and numerical simulations [5–7] have been conducted on the thermocapillary convection in the LEC system or in the bilayer system. Liu and Roux [8] performed numerical simulations to study the pure thermocapillary convection in the system composed of two immiscible liquid layers with a horizontal temperature gradient. Their results indicated that the encapsulation with high viscosity and low thermal diffusivity may significantly reduce the convection in the lower layer. Similar results were also reported by Gupta et al. [9,10] through a series of numerical simulations in a differentially heated rectangular cavity. Moreover, Madruga et al. [11,12] extended investigations to the stability of thermocapillary convection in an infinite horizontal two-layer system bounded by two solid boundaries on the top and bottom and predicted three types of flow instabilities. Nepomnyashchy and Simanovskii [13] investigated the two-layer system composed of 5cS silicone oil and HT-70 with a horizontal temperature gradient. For large values of Marangoni number and Grashof number, an oscillatory instability was developed.

The effect of system rotation on thermocapillary convection in a two-layer system was taken into account in only few published

* Corresponding author.
E-mail address: shiwy@cqu.edu.cn (W.-Y. Shi).

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reports. Numerical simulations of flow field in LEC configuration by Fontaine et al. [14] suggested that large crystal rotation rate suppressed the time-dependent flow driven by buoyancy and rotation but thermocapillary force was not taken into account in their work. Wu and Li [15] investigated the effect of the counter rotation of crucible and crystal in a LEC configuration when the coupled thermocapillarity, centrifugal force and Coriolis force were considered during the investigations. Their results revealed that the crystal rotation could suppress the flow instability while the crucible rotation had an opposite effect.

Although thermocapillary convection in bilayer system has been investigated by numerous works, there is actually lack of experimental report on the wave pattern of the oscillatory thermocapillary convection due to the limitation of observation method for bilayer system. The stability analysis or two-dimensional simulation conclusion can't be simply extrapolated into the three-dimensional nonlinear regime [16]. The characteristics of the wave pattern of the oscillatory thermocapillary convection in bilayer system is thus still an open question up to now. In this work, we have developed the computer codes for two-layer system based on our previous version for single-layer [17] and have conducted a series of three-dimensional simulations to investigate the characteristics of the oscillatory thermocapillary convection in a two-layer pool with and without system rotation. The critical condition for the onset of hydrothermal waves and its patterns as well as the mechanism which causes the flow instability have been investigated carefully.

2. Models and numerical methods

2.1. Physical and mathematical models

We consider two immiscible liquids in an annular pool. The thickness of lower layer and upper layer are h_1 and h_2, and the inner and outer radius are r_i and r_o, respectively. The annular pool rotates around its central axis with a constant angular velocity Ω. The aspect, radius and thickness ratios are respectively defined as $A = \Delta r/h_1 (\Delta r = r_o - r_i)$, $r^* = r_i/r_o$ and $h^* = h_2/h_1$ and we assign these parameter values as $A = 4$, $r^* = 0.5$ and $h^* = 1$ in the present work.

The outer wall is maintained at a higher temperature T_o while the inner wall at a lower temperature T_i. The annular pool is filled with 5cS silicone oil as upper layer liquid and HT-70 as lower layer liquid. Their thermophysical properties refer to Refs. [11,13]. For concise, the liquid–liquid interface is shortly called interface and the top free surface or liquid–gas interface is shortened to surface hereafter. The liquids are assumed to be incompressible Newtonian liquid with constant properties except for the temperature dependence of surface tension and interface tension. Thus the Marangoni effect acts on both the surface and interface. The rigid bottom and the surface are considered to be adiabatic. The flow is considered to be laminar. The surface and interface are assumed to be flat and non-deformable.

Under the assumptions above, the mathematical model in the absence of gravity is expressed by the following dimensionless governing equations in a cylindrical rotational coordinate system co-rotating with pool around the central Z axis.

$$\nabla \cdot \boldsymbol{V}_i = 0 \tag{1}$$

$$\frac{\partial \boldsymbol{V}_i}{\partial \tau} + \boldsymbol{V}_i \cdot \nabla \boldsymbol{V}_i = -\frac{\rho_1}{\rho_i}\nabla P_i + \frac{\nu_i}{\nu_1}\nabla^2 \boldsymbol{V}_i - 2Ta\boldsymbol{e}_z \times \boldsymbol{V}_i \tag{2}$$

$$\frac{\partial \Theta_i}{\partial \tau} + \boldsymbol{V}_i \cdot \nabla \Theta_i = \frac{\alpha_i}{\alpha_1}\frac{1}{Pr}\nabla^2 \Theta_i \tag{3}$$

The boundary conditions are written as follows:

at the surface ($r_i/\Delta r < R < r_o/\Delta r$, $Z = (h_1 + h_2)/\Delta r$, $0 \leqslant \theta < 2\pi$):

$$\mu^* \frac{\partial U}{\partial Z} = -\gamma_T^* \frac{Ma}{Pr}\frac{\partial \Theta}{\partial R}, \quad \mu^* \frac{\partial V}{\partial Z} = -\gamma_T^* \frac{Ma}{Pr}\frac{\partial \Theta}{R\partial \theta}, \quad W = 0, \quad \frac{\partial \Theta}{\partial Z} = 0; \tag{4a-4d}$$

at the interface ($r_i/\Delta r < R < r_o/\Delta r$, $Z = h_1/\Delta r$, $0 \leqslant \theta < 2\pi$):

$$\left.\frac{\partial U}{\partial Z}\right|_1 - \mu^* \left.\frac{\partial U}{\partial Z}\right|_2 = -\frac{Ma}{Pr}\frac{\partial \Theta}{\partial R}, \quad \left.\frac{\partial V}{\partial Z}\right|_1 - \mu^* \left.\frac{\partial V}{\partial Z}\right|_2 = -\frac{Ma}{Pr}\frac{\partial \Theta}{R\partial \theta},$$
$$W = 0, \quad \left.\frac{\partial \Theta}{\partial Z}\right|_1 = \lambda^* \left.\frac{\partial \Theta}{\partial Z}\right|_2; \tag{5a-5d}$$

at the bottom ($r_i/\Delta r < R < r_o/\Delta r$, $Z = 0$, $0 \leqslant \theta < 2\pi$):

$$U = V = W = 0, \quad \frac{\partial \Theta}{\partial Z} = 0; \tag{6a-6d}$$

at the cold inner wall ($R = r_i/\Delta r$, $0 \leqslant Z \leqslant (h_1 + h_2)/\Delta r$, $0 \leqslant \theta < 2\pi$):

$$U = V = W = 0, \quad \Theta = 0; \tag{7a-7d}$$

at the hot outer wall ($R = r_o/\Delta r$, $0 \leqslant Z \leqslant (h_1 + h_2)/\Delta r$, $0 \leqslant \theta < 2\pi$):

$$U = V = W = 0, \quad \Theta = 1; \tag{8a-8d}$$

the initial conditions adopted in our simulations are ($\tau = 0$, $r_i/\Delta r \leqslant R \leqslant r_o/\Delta r$, $0 \leqslant Z \leqslant (h_1 + h_2)/\Delta r$, $0 \leqslant \theta < 2\pi$):

$$U = V = W = 0, \quad \Theta = \frac{\ln(r/r_i)}{\ln(r_o/r_i)}; \tag{9a-9d}$$

where the variables in the lower layer and upper layer are marked by the subscript 1 and 2, respectively. The length, time, pressure and velocity are scaled by Δr, $\Delta r^2/\nu_1$, $\nu_1\mu_1/\Delta r^2$ and $\nu_1/\Delta r$, respectively. The reduced temperature Θ is defined as $\Theta = (T - T_i)/(T_o - T_i)$ and the asterisks represent the ratios of physical property of these two liquids, e.g., $\mu^* = \mu_2/\mu_1$, $\gamma_T^* = \gamma_{T2}/\gamma_{T1-2}$. Where ν is the kinetic viscosity; α the thermal diffusivity; λ the thermal conductivity; γ_{T1-2} and γ_{T2} the temperature dependence of interface tension and surface tension; $\boldsymbol{e}_z$ a unit vector in positive axial direction. The Prandtl, Marangoni and Taylor numbers in the fundamental equations are defined based on the properties of the lower layer as $Pr = \nu_1/\alpha_1$, $Ma = \gamma_{T1-2}(T_o - T_i)\,\Delta r/\mu_1\alpha_1$ and $Ta = \Omega\Delta r^2/\nu_1$.

2.2. Numerical method for solving non-linear equations

The transient Eqs. (1)–(9) are discretized by the finite volume method in a non-uniform staggered grid. The numerical method is the same as that in our previous work [17]. The dimensionless computation time step ranges from 3.75×10^{-6} to 1.25×10^{-5}. At each time step, the computation converges when the maximum absolute dimensionless residual error of continuity equation among all of the control volumes is less than 10^{-6} and the maximum relative variation of variables is less than 10^{-4}.

The non-uniform grid of $80^R \times 40^Z \times 100^\theta$ is used in the present work. Moreover, the numerical code is verified by comparing our result with $A = 4$, $r^* = 0.99$ and $h^* = 1$ to the analytical solution of Doi and Koster [7]. The radial velocity along axial direction have a good quantitative correspondence with the maximum deviation of 1.2% on the surface. Thus a conclusion can be drawn that the code is correct.

3. Results and discussion

3.1. Basic flow

When Ma is small, the thermocapillary flow is axisymmetric and steady. Hereafter, we call this steady axisymmetric flow as "basic flow".