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Technical Note

Flow pattern transition of thermal–solutal capillary convection with the capillary ratio of −1 in a shallow annular pool

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ABSTRACT

In order to understand the flow pattern transition processes, a series of three-dimensional numerical simulations for thermal–solutal capillary convection in an annular pool subjected to simultaneous radial temperature and solutal concentration gradients were conducted. The capillary ratio was fixed at −1. The working fluid was the toluene/n-hexane mixture with the Prandtl number of 5.54 and the Schmidt number of 142.8. Results show that there exists a quiescent conductive state in the liquid pool when thermocapillary Reynolds number is small. With the increase of thermocapillary Reynolds number, the flow bifurcates orderly into three different kinds of the oscillatory flows, i.e., the travelling wave, the combined travelling wave with stationary wave, and the vibrating spoke pattern. The oscillatory frequency increases monotonously for the travelling wave and the combined travelling wave with stationary wave. Furthermore, the wave number is independent of the thermocapillary Reynolds number. These multiple complicated flow patterns are due to the different distributions of the local capillary ratio along the free surface.

1. Introduction

The crystal growth theory always links to the thermodynamics and hydrodynamics, which can be regarded as the cornerstone of the crystal growth technology [1]. So far, many investigations on the melt flow in the single crystal growth have been performed systematically [2,3]. Recently, double-diffusive convection and thermal–solutal capillary convection relating to the binary crystal growth also attract an increasing attention.

Double-diffusive convection is driven by the coupled thermal and solutal buoyancy forces. The early investigations on double-diffusive convection are motivated by oceanography and the later applications in crystal growth, alloy solidification and casting [4,5]. A special case is that the induced thermal and solutal buoyancy forces are opposite and of equal magnitude, i.e., buoyancy ratio $R_\rho = -1$. In this case, whether the directions of the temperature and concentration gradients are vertical or horizontal, there exists a quiescent equilibrium corresponding to the pure conductive state. Gobin and Bennacer [6] performed a stability analysis of double-diffusion convection in a vertical fluid layer and claimed that the critical Rayleigh number is a function of the Lewis number but independent on the Prandtl number. Bergeon and Knobloch [7] found a complex flow state with the finite amplitude nonlinear oscillation by numerical simulation. This kind of the flow seems to be either periodic or chaotic. In the following decades, this issue has been investigated systematically by utilizing bifurcation analyses, stability analyses and numerical simulation [8–11].

In the binary melt with a free surface, the capillary forces depend on the temperature and solute concentration distributions along the free surface. When the capillary ratio is $R_\sigma = -1$, the solutal and thermal capillary effects are equal and opposite. In this case, the quiescent state in the liquid layer has been certified [12–14]. The Hopf bifurcation from steady state to periodical oscillatory state, reverse transitions from oscillatory flow to quiescent equilibrium and from chaotic flow to steady one have been predicted [13,14]. Furthermore, different routes of flow evolution were also exhibited [15]. On the other hand, Yu et al. [16] found that the solutal concentration gradient induced by the temperature gradient has slightly effect on the travelling waves.

It's worth mentioning that the annular geometry meets the requirement of a large spatial extension for travelling waves to establish them azimuthally. The oscillatory thermocapillary flow in an annular pool is usually characterized by travelling waves i.e. the "hydrothermal waves" (HTWs) [3]. Li et al. [17,18] discussed the mechanisms of the convective instabilities and the critical conditions for the onset of the oscillatory thermocapillary flow in the annular pool. It was found that the azimuthal velocity of the

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HTWs and the amplitude of the temperature fluctuation increase with the radial temperature gradient. However, there are few reports that are paying attention to the coupled thermal and solutal capillary convection in a shallow annular pool subjected to simultaneous radial thermal and solutal gradients. The present work aims mainly at the flow pattern transition of the coupled thermal–solutal capillary convection and the destabilization mechanism.

2. Physical and mathematical model

2.1. Basic assumptions and governing equations

The physical model is annular pool that the inner radius, outer radius and depth of the annular pool are respectively marked as r_i, r_o and d. The radius ratio is defined as $\eta = r_i/r_o$, while the aspect ratio is $\varepsilon = d/(r_o - r_i)$. At the cylindrical sidewalls, distinguishing temperatures T_o and T_i, concentrations C_o and C_i are allocated, where $T_o > T_i$ and $C_o > C_i$.

Assumptions for the simplification are based on the Refs. [12–14]. It is suggested that the flow is laminar. The nondeformable free surface and the bottom wall of the annular pool are perfectly adiabatic and impermeable. The no-slip boundary condition is applied for all the solid walls. The binary fluid is assumed to be an incompressible Newtonian fluid with constant physical properties except for the surface tension. The Soret effect, the Dufour effect and the viscous dissipation have been neglected. On the free surface, the capillary boundary condition is taken into consideration and the surface tension is the linear function of the temperature and concentration. By applying $(r_o - r_i)$, $(r_o - r_i)^2/\nu$, $\nu/(r_o - r_i)$ and $\rho\nu 2/(r_o - r_i)^2$ as the reference scales for length, time, velocity and pressure respectively, the dimensionless governing equations can be expressed as:

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

$$\frac{\partial \boldsymbol{V}}{\partial \tau} + \boldsymbol{V} \cdot \nabla \boldsymbol{V} = -\nabla P + \nabla^2 \boldsymbol{V}, \tag{2}$$

$$\frac{\partial \Theta}{\partial \tau} + \boldsymbol{V} \cdot \nabla \Theta = \frac{1}{Pr} \nabla^2 \Theta, \tag{3}$$

$$\frac{\partial \Phi}{\partial \tau} + \boldsymbol{V} \cdot \nabla \Phi = \frac{1}{Sc} \nabla^2 \Phi. \tag{4}$$

where $\boldsymbol{V} = \boldsymbol{V}(V_R, V_\theta, V_Z)$ denotes the dimensionless velocity vector, ν kinematic viscosity, $\Theta = (T - T_i)/(T_o - T_i)$ the dimensionless temperature and $\Phi = (C - C_i)/(C_o - C_i)$ the dimensionless concentration.

Under the assumptions and definitions above, the boundary conditions at the free surface are expressed as follows:

$$PV_Z = 0,\ \frac{\partial V_R}{\partial Z} = -Re_T \frac{\partial \Theta}{\partial R} - Re_C \frac{\partial \Phi}{\partial R},$$
$$\frac{\partial V_\theta}{\partial Z} = -Re_T \frac{\partial \Theta}{R \cdot \partial \theta} - Re_C \frac{\partial \Phi}{R \cdot \partial \theta},\ \frac{\partial \Phi}{\partial Z} = \frac{\partial \Theta}{\partial Z} = 0 \tag{5a-d}$$

The initial conditions are expressed as follows ($\tau = 0$):

$$V_R = V_\theta = V_Z = 0,\ \Theta = \Phi = -\ln[R(1-\eta)/\eta]/\ln \eta. \tag{6a-b}$$

The thermal and solutal capillary Reynolds numbers, and the capillary ratio are respectively defined as:

$$Re_T = \frac{\gamma_T \Delta T (r_o - r_i)}{\mu \nu},\ Re_C = \frac{\gamma_C \Delta C (r_o - r_i)}{\mu \nu},$$
$$R_\sigma = \frac{Re_C}{Re_T} = \frac{\gamma_C \Delta C}{\gamma_T \Delta T} = -1. \tag{7a-c}$$

where $\Delta T = T_o - T_i$ and $\Delta C = C_o - C_i$. γ_T and γ_C are temperature and solutal coefficients of surface tension, respectively. μ is dynamic viscosity of the working fluid.

In the present work, the capillary ratio, the aspect ratio and the radius ratio of the annular pool are respectively fixed at $R_\sigma = -1$, $\varepsilon = 0.15$ and $\eta = 0.5$. The working fluid is the toluene/n-hexane solution with an average toluene mass fraction of $C_0 = 0.2627$. The thermophysical properties of the toluene/n-hexane solution come from Refs. [19–22].

2.2. Numerical method and mesh validation

The governing equations and the boundary conditions are discretized by using the finite volume method and solved by the SIMPLEC algorithm [13,14]. The central-difference approximation is applied for the diffusion terms while the QUICK scheme is used for the convection terms. In order to ensure the accuracy, the small dimensionless time steps of $(0.6–1.2) \times 10^{-4}$ are chosen. It is proved that the iteration residual error of 10^{-4} is accurate enough for the present simulations.

The nonuniform mesh of $80^R \times 200^\theta \times 25^Z$ is used. Moreover, the numerical method has been validated by comparing with simulation results of thermal–solutal capillary convection in the cubic cavity that was performed by Zhan et al. [14]. The similar flow patterns, the temperature and concentration fields have been reproduced. The maximum deviation of Nusselt (Nu) numbers is less than 2.3%.

3. Results and discussion

In this work, the coupled thermal–solutal capillary convection of the binary solution with the moderate Prandtl number of $Pr = 5.54$ and Lewis number of $Le = 25.28$ in the annular pool at the capillary ratio of $R_\sigma = -1$ has been carefully investigated at a wide range of thermocapillary Reynolds number. With the increase of thermocapillary Reynolds number, various flow patterns are exhibited as follows.

3.1. Quiescent equilibrium (QE)

When thermocapillary Reynolds number is small, there exists a quiescent equilibrium state in the liquid pool up to $Re_T = 915$. When the thermocapillary and solutocapillary forces are of equal magnitude and contrary direction, two capillary effects are balanced each other. This quiescent equilibrium state has been discussed in Bergman's original work [12]. Furthermore, according to the linear stability analysis of the thermal–solutal capillary convection in a cavity performed by Chen et al. [13], the motionless equilibrium state loses its stability due to small disturbances and then bifurcates to oscillatory flow at $Re_T = 362$.

3.2. Three-dimensional oscillatory flow

When the thermocapillary Reynolds number is large enough, three-dimensional (3D) oscillatory flows appear in the liquid pool. In this case, the flow pattern depends mainly on the revised thermal capillary Reynolds number Re_T^i, solutal capillary Reynolds number Re_C^i and capillary ratio R_σ^i, which are defined as

$$Re_T^i = \frac{\gamma_T (r_o - r_i)^2}{\mu \nu} \left(\frac{\partial T}{\partial r}\right)^i,\ Re_C^i = \frac{\gamma_C (r_o - r_i)^2}{\mu \nu} \left(\frac{\partial C}{\partial r}\right)^i,\ Re_\sigma^i = \frac{Re_C^i}{Re_T^i}, \tag{8a-c}$$

where $(\partial T/\partial r)^i$ and $(\partial C/\partial r)^i$ are the local temperature and solute concentration gradients along the radial direction on the free surface.