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Effect of capillary ratio on thermal-solutal capillary-buoyancy convection in a shallow annular pool with radial temperature and concentration gradients

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ABSTRACT

In order to understand the effect of capillary ratio on the thermal-solutal capillary-buoyancy convection in an annular pool subjected to simultaneous radial thermal and solutal gradients, a series of three-dimensional direct numerical simulations have been carried out. The working fluid was the toluene/*n*-hexane mixture fluid with the Prandtl number of 5.54 and the Schmidt number of 142.8. The capillary ratio R_σ varied from −0.8 to 0.2. Results show that the flow is axisymmetric and steady at small thermocapillary Reynolds number. Four types of such two-dimensional steady flow, i.e., counter-clockwise unicellular flow, clockwise unicellular flow, flows with two separate cells stratified horizontally and vertically, appear with the variations of capillary ratio and thermocapillary Reynolds number. With the further increase of thermocapillary Reynolds number, two-dimensional steady flow bifurcates firstly to three-dimensional steady flow at the first critical thermocapillary Reynolds number, then to three-dimensional oscillatory flow at the second critical thermocapillary Reynolds number. When the three-dimensional oscillatory flow appears, the temperature and concentration fluctuations on the free surface are indicated as either the coexistence of “hydro-thermal wave” and “hydro-solutal wave”, or the “vibrating straight spokes”. A reverse transition from periodic flow to steady flow is encountered.

1. Introduction

The thermal-solutal capillary-buoyancy convection usually takes place in a mixture liquid layer with free surface under the combined effects of capillary and buoyancy forces, which are induced by the temperature and solute concentration gradients. This convection is important in many industrial applications, especially for crystal growth of compound semiconductors and solidification of alloy castings and ingots [1]. During crystal growth and solidification, the flow instability of the solution or the melt in the crucible is one of the important factors that affect the compositional uniformity and the growth morphology of the solid/liquid interface [2]. In order to obtain the high-quality crystal and alloy products, the thermal-solutal capillary-buoyancy convection in the crucible must be well controlled. The flow pattern transition and the instability mechanism of thermal-solutal capillary convection must be well understood.

The investigation on thermal-solutal capillary-buoyancy convection in the process of crystal growth of compound semiconductor has been carried out extensively. Okano et al. [2] performed the numerical simulation on the oscillatory behavior of the melt during the melting of GaSb/InSb/GaSb alloy in the horizontal Bridgman configuration. They pointed out that the thermal-solutal capillary effect should be responsible for oscillatory flow, which may lead to growth striations and finally lower the quality of the crystal. Arafune et al. [3] experimentally demonstrated that the solutocapillary convection can suppress or enhance the thermocapillary convection during the growth of InSb crystal in the horizontal Bridgman liquid pool [4]. Cröll et al. [5] experimentally investigated the solutocapillary convection during the growth of germanium-silicon crystal in a rectangular graphite crucible on the ground and under microgravity. Results show that the flow intensity under microgravity is generally greater than that under normal gravity due to the depressing effect of solutal buoyancy convection. Additionally, many numerical and experimental results also show that melt turbulence and thermal fluctuations in the process of crystallization and solidification can be effectively suppressed by the transverse magnetic field [6–8].

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Nomenclature

Bo	Bond number
C	mass fraction of toluene
C_p	specific heat capacity, J/(kg K)
d	depth, m
D	mass diffusivity of species, m^2/s
F	dimensionless frequency
Gr	Grashof number
Le	Lewis number, $Le = \alpha/D$
m	wave number
P	dimensionless pressure
Pr	Prandtl number, $Pr = \nu/\alpha$
r	radius, m
R	dimensionless radius
Re	Reynolds number
R_σ	capillary ratio, Eq. (13a)
R_ρ	buoyancy ratio, Eq. (13b)
Sc	Schmidt number, $Sc = \nu/D$
T	temperature, °C
v	velocity, m/s
$\boldsymbol{V}$	dimensionless velocity vector
z	axial coordinate, m
Z	dimensionless axial coordinate

Greek symbols

α	thermal diffusivity, m^2/s
β	expansion coefficient
ε	aspect ratio, $d/(r_o - r_i)$
Φ	dimensionless concentration, $\Phi = (C - C_i)/(C_o - C_i)$
γ	coefficient of surface tension
η	radius ratio, $\eta = r_i/r_o$
μ	dynamic viscosity, kg/(m s)
ν	kinematic viscosity, m^2/s
Θ	dimensionless temperature, $\Theta = (T - T_i)/(T_o - T_i)$
ρ	density, kg/m^{-3}
σ	surface tension, N/m
τ	dimensionless time
ψ	dimensionless stream function

Subscripts

ave	average
c	critical
C	solutal
i	inner wall
o	outer wall
p	period
R, Z, θ	coordinate directions
T	thermal

For the horizontal layer of a binary mixture subjected to vertical temperature and solute concentration gradients, Warmuziński and Tańczyk [9] carried out linear analysis on the coupled thermal-solutal capillary-buoyancy convection in the acetone/methanol mixture film. They determined the critical values for the bifurcations of oscillatory and stationary convections and analyzed the analogy between the heat and mass transfer. Chen and Su [10] concluded that the Prandtl number and Lewis number have a profound effect on stability characteristics of the flow at low gravity conditions. McTaggart [11] predicted that when the effect of buoyancy force is ignored, the destabilized convection at the onset of instability can be oscillatory or stationary, depending on whether the thermocapillary and solutocapillary forces enhance or counteract each other. Tanny et al. [12] performed experimental visualization of flow pattern by schlieren method in a rectangular tank with the vertical temperature and concentration gradients. Results showed that the first instability onset is of the Marangoni type. Well-organized small plumes emerged and persisted close to the top free surface. Nevertheless, when the thermal Rayleigh number is large enough, the small plumes evolve into larger double-diffusive plumes. Chan and Chen [13] experimentally and numerically investigated the interactive effects of thermal-solutal capillary and buoyancy forces in a rectangle tank filled with vertical stratified ethanol-water solution. Finger convection caused by thermal and solutal capillary motion was observed. Besides, many researchers have discussed the Soret effect on the Marangoni instability in the thin infinite layers [14,15] and confined cavities [16]. A diversity of instability modes has been revealed.

The flow stability of the binary mixture layer subjected to simultaneous horizontal thermal and concentration solutal gradients is different from that subjected to vertical gradients. Jue [17] numerically analyzed the thermal-solutal capillary-buoyancy convection in a cavity when the capillary ratio (the ratio of soluto-capillary effect to thermocapillary effect) ranges from 0 to −1 and the buoyancy ratio (the ratio of solutal buoyancy effect to thermal buoyancy effect) is fixed at −5. Results show that the thermal-solutal capillary effect on the free surface alters the evolution of the flow pattern and influences the local heat and mass transfer rates. Furthermore, he also found that the flow patterns of the surface-tension-driven convections are similar to those of the lid-driven cavity flows. Al-Amiri et al. [18] numerically investigated the steady lid-driven convection in a square cavity filled with a binary fluid. It was found that the opposite thermal and solutal buoyancy forces slow down the main vortex and lead to the formation of two prime vortices. Chen and Chan [19] performed the linear stability analysis on the combined effects of buoyancy and capillary forces**.** The critical conditions for the onset of salt-finger instability and travelling wave instability were carefully determined.

In the previous investigations, either the thermal convection with zero concentration difference [20–22], or the surface-tension-driven convection under zero gravity condition [23,24] has been systematically investigated in the annular pool models. Moreover, Yu et al. [25,26] numerically investigated the thermal capillary-buoyancy convection with Soret effect in a shallow annular pool filled with binary mixture. It was found that the influence of the Soret effect on the flow instability is slight. However, much less work has been devoted to the quantitative analysis of the effect of capillary ratio R_σ on the thermal-solutal capillary-buoyancy convection in the annular pool. Therefore, in this paper, a series of three-dimensional numerical simulations have been conducted to illustrate the flow characteristics and flow pattern transition.

2. Physical and mathematical model

2.1. Basic assumptions and governing equations

As shown in Fig. 1, the annular pool is filled with binary fluid with a horizontal and nondeformable free surface. Its inner radius, outer radius and depth are respectively marked as r_i, r_o and d. The