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ORIGINAL ARTICLE

Moderate Prandtl Number Nanofluid Thermocapillary Convection Instability in Rectangular Cavity

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Abstract
Thermocapillary convection of moderate Prandtl number nanofluid in rectangular cavity is numerically investigated in this paper, and the effect of nanoparticle volume fraction on flow instability is analyzed. The computational results show that, the critical temperature difference deceases gradually with nanoparticle volume fraction increasing, and nanofluid thermocapillary convection is less stable than the base fluid. With the increase of nanoparticle volume fraction the velocity oscillatory amplitude decreases, but the oscillatory period increases. Nanofluid oscillatory thermocapillary convection has one dominant oscillation frequency, and with nanoparticles volume fraction increasing the second fundamental frequency strengthens gradually.

Keywords Nanofluids · Thermocapillary convection · Flow instability · Critical temperature difference

Abbreviations

C_p	specific heat, J/kgK
h	cavity height, m
l	cavity length, m
P	pressure, Pa
Pr	Prandtl number, $Pr = C_p\mu/\lambda$
T	fluid temperature, K
t	time, s
V	velocity vector, m/s
u	x-velocity, m/s
v	y-velocity, m/s
x	x-direction coordinate, m
y	y-direction coordinate, m

Greek symbols

λ	thermal conductivity, W/mK
ν	kinematic viscosity, m^2/s
α_p	nanoparticles volume fraction
μ	dynamic viscosity, kg/ms
ρ	density, kg/m^3
τ	oscillatory period, s

Subscripts

f	base fluid
nf	nanofluid
p	nanoparticles
h	hot wall
c	cold wall

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Introduction

Thermocapillary convection extensively exists in microgravity environment and many industrial processes, e.g. crystal growth, and film coating, etc. This flow is driven by temperature gradient at liquid free surface. Thermocapillary convection instability first reported by Smith and Davis, thereafter, the flow transition and instability characteristics are extensively investigated by many investigators (Yu et al. 2015a, 2015b; Shi et al. 2017; Yang et al. 2017; Zhou et al. 2016; Zhou and Huai 2015a, 2015b). Nanofluids is a complex fluid with high thermal conductivity, and it can be obtained by non-metal or metal nanoparticles uniformly dispersed in water, alcohol or oil. Since the concept of nanofluids was first proposed by Choi (Choi 1995), the nanofluid has been used in many occasions, and nanofluid thermocapillary convection exists in heat pipe, boiling heat transfer, biomedicine and other fields (Susanta 2017; Wu et al. 2020; Naveen et al.

2018; Du et al. 2019; Stetten et al. 2018). Therefore, the flow characteristics and instability of nanofluid thermocapillary convection has attracted researchers' attention in recent years. Aminfar et al. (Aminfar et al. 2012) reported the nanofluids thermocapillary-buoyancy convection in a float zone for the first time, and their computational results showed that the increase of nanofluids volume fraction can influence the flow characteristics of thermocapillary convection. Saleh and Hashim (Saleh and Hashim 2015) carried out numerical studies on steady buoyancy-Marangoni convection in a rectangular cavity, and obtained the influence of Marangoni number on flow and Nusselt number. Al-Sharafi et al. (Al-Sharafi et al. 2016) studied the flow and heat transfer characteristics of water-carbon nanotube nanofluids Marangoni convection in a droplet. The authors (Jiang and Xu 2017) studied nanofluids steady thermocapillary convection by numerical simulation, and the effect of nanoparticles on thermocapillary convection flow and heat transfer was revealed. Kolsi et al. (Kolsi et al. 2017) numerically investigated steady buoyancy-thermocapillary convection flow characteristics and entropy generation distribution of nanofluids in a three-dimensional cavity. The results showed that the heat transfer capacity increases with the increase of nanoparticles volume fraction, and the total entropy production also increases. Sheikholeslami et al. (Sheikholeslami and Chamkha 2017) investigated the effect of MHD effect on steady-state Marangoni convection of nanofluids. Abdullah et al. (Abdullah et al. 2018) carried out linear stability analysis of nanofluids Marangoni convection in thin liquid layer under vertical temperature difference, and the effects of nanoparticles volume fraction and dimension on the stability were analyzed. Gevorgyan et al. (Gevorgyan et al. 2017) experimentally studied the velocity variation characteristics of Marangoni effects driven flow when nanofluid surface is heated by laser, and the influence of light intensity and nanoparticles concentration on flow was studied. The entropy production of the steady-state buoyancy-Marangoni convection in a three-dimensional homogeneous porous medium was studied by Zhuang and Zhu (Zhuang and Zhu 2018), the effect of nanoparticles volume fraction on the entropy production was discussed. Recently, the authors (Jiang and Zhou 2019) further studied nanofluid surface tension driven flow, which the influence of nanoparticles on surface tension was considered.

The above research works show that the investigators mainly focus on the steady flow characteristics of nanofluid thermocapillary, however, there is still no relevant report on flow instability. It is well known that, nanofluid is a two-phase mixture fluid and its macroscopic physical properties such as dynamic viscosity and thermal conductivity is different from that of the base fluid. Meanwhile, the random Brownian motion of nanoparticles can enhance the energy and momentum transfer between nanoparticles and the base fluid. So, the transition condition and instability characteristics of nanofluid thermocapillary convection may different from that of single-phase fluid, and at present these problems have not been fully revealed. Therefore, the purpose of the paper is to study the nanofluid thermocapillary convection instability, and clarify the effect of nanoparticle volume fraction on critical temperature difference and flow characteristics.

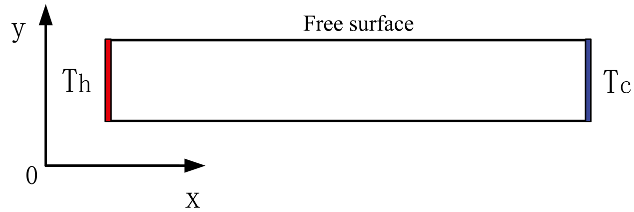

Fig. 1 Physical model

Physical and Mathematical Model

In order to study the instability of thermocapillary convection, a differentially heated rectangular cavity is a widely used research model, so this classical model is also used in this paper. Figure 1 depicts a two-dimensional rectangular cavity with a length (l) of 20 mm and height (h) of 3 mm, which is filled with silicon oil. The right and left walls are differentially heated, and the temperature of the left and right walls are T_h and T_c respectively. The free surface and the bottom wall are considered to be adiabatic. Under the action of horizontal temperature gradient, thermocapillary convection driven by surface tension gradient is formed in the cavity. In order to investigate the nanofluid thermocapillary convection instability, the convection is assumed to be incompressible laminar flow due to the small temperature difference. Thermophysical properties of the base fluid except for surface tension keep constant, and surface tension is a linear function of temperature. Due to the depth of liquid layer is very small the buoyancy effect is ignored in our investigation. The initial temperature and flow fields in the cavity are $T = T_c$ and $\vec{V}=0$, respectively. Then, the governing equations of nanofluid thermocapillary convection in this two-dimensional cavity can be written as follows:

Continuity equation:

$$\nabla \cdot \vec{V} = 0 \tag{1}$$

Momentum equation:

$$\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} = -\frac{1}{\rho_{nf}} \nabla p + \frac{\mu_{nf}}{\rho_{nf}} \nabla^2 \vec{V} \tag{2}$$

Table 1 Thermophysical parameters of base fluid and nanoparticles

Thermal properties Base fluid and particles	ρ(kg/m^3)	c_p(J/kgK)	λ(W/m K)	μ(m^2/s)	γ_T(N/m K)	Pr
Base fluid (silicon oil)	760	1380	0.1	-5.01 × 10^{-4}	-6.4 × 10^{-5}	10
Nanoparticles (Copper)	8978	381	387.6	/	/	/

Energy equation:

$$\frac{\partial T}{\partial t} + \vec{V} \cdot \nabla T = \frac{\lambda_{nf}}{\rho_{nf} cp_{nf}} \nabla^2 T \tag{3}$$

where $\vec{V}$ is the velocity vector, T is the temperature, t is time, p is the pressure, ρ is density, λ is the thermal conductivity, and μ is the dynamic viscosity, and the subscript *nf* denotes nanofluid.

Thermophysical Properties of Nanofluids

The determination of thermophysical properties of nanofluids is significantly important for the numerical investigation. In the present paper, the equations of density and specific heat of nanofluids are as follows:

$$\rho_{\mathrm{nf}} = \alpha_p \rho_p + \left(1 - \alpha_p\right) \rho_f \tag{4}$$

$$(\rho cp)_{nf} = \alpha_p \left(\rho c_p\right)_p + \left(1 - \alpha_p\right) \left(\rho c_p\right)_f \tag{5}$$

The Eq. (4) is nanofluid density equation, which is according to the mixture rule as suggested in Ref. (Das et al. 2008). The Eq. (5) is specific heat equation, and this is based on the assumption of thermal equilibrium between the nanoparticles and the base fluid (Khanafer and Vafai 2011).

Thermal conductivity of nanofluid (Hamilton and Crosser 1962):

$$\lambda_{nf} = \lambda_f \left[\frac{\left(\lambda_p + 2\lambda_f\right) - 2\alpha_p \left(\lambda_f - \lambda_p\right)}{\left(\lambda_p + 2\lambda_f\right) + \alpha_p \left(\lambda_f - \lambda_p\right)} \right] \tag{6}$$

Dynamic viscosity of nanofluid (Brinkman 1952):

$$\mu_{nf} = \frac{\mu_f}{\left(1 - \alpha_p\right)^{2.5}} \tag{7}$$

where α_p is nanoparticle volume fraction. The subscript f represents the base fluid, the subscript *p* represents the nanoparticles, and the subscript *nf* represents the nanofluid.

Boundary Conditions

The boundary conditions of surface tension driven convection in a rectangular cavity are as follows:

$$\mathrm{u} = \mathrm{v} = 0, \mathrm{T} = T_c \text{ at } x = 0 \tag{8}$$

$$\mathrm{u} = \mathrm{v} = 0, \mathrm{T} = T_h \text{ at } x = l \tag{9}$$

$$\mathrm{u} = \mathrm{v} = 0, \frac{\partial T}{\partial y} = 0 \text{ at } y = 0 \tag{10}$$

$$\mu \frac{\partial u}{\partial y} = -\gamma_T \frac{\partial T}{\partial x}, \mathrm{v} = 0, \frac{\partial T}{\partial y} = 0 \text{ at } y = h \tag{11}$$

where u and v are the velocity components in the x- and y-directions, respectively.

The Thermophysical Parameters of Nanofluid

In the numerical simulations, the base fluid is silicon oil and the nanoparticle is copper. The thermophysical parameters of the base fluid and nanoparticles are shown in Table 1.

Computational Method

The governing equations are discretized by the finite volume method, in which the discretization of convective terms is by QUICK format and the diffusion terms by second order central difference schemes. The PISO algorithm is used to solve the pressure–velocity coupling. In the process of numerical calculation, when the velocity, temperature and pressure of the main parameters of the relative rate of change are less than 10^{-5} the solution is assumed to be converged. The validity of computational code can refer to our previous published paper (Jiang et al. 2021, 2020; Jiang and Zhou 2020). The grid used in this work is a non-uniform orthogonal mesh, and the mesh is locally refined in all the wall and free surface regions. Grids of 100 × 30, 150 × 40, 200 × 50 and 250 × 70 are tested, and the average oscillatory period of thermocapillary convection under different grid numbers is illustrated in Table 2, which shows that grid 200 × 50 is sufficient for the numerical simulation of nanofluid thermocapillary convection.

Table 2 Average oscillatory period under different grids (Silicon oil-Cu, α_p = 0.05 $\Delta T = 2K$)

Grid numbers	Average oscillatory period (s)
100 × 30	29.81
150 × 40	29.02
200 × 50	28.57
250 × 70	28.50

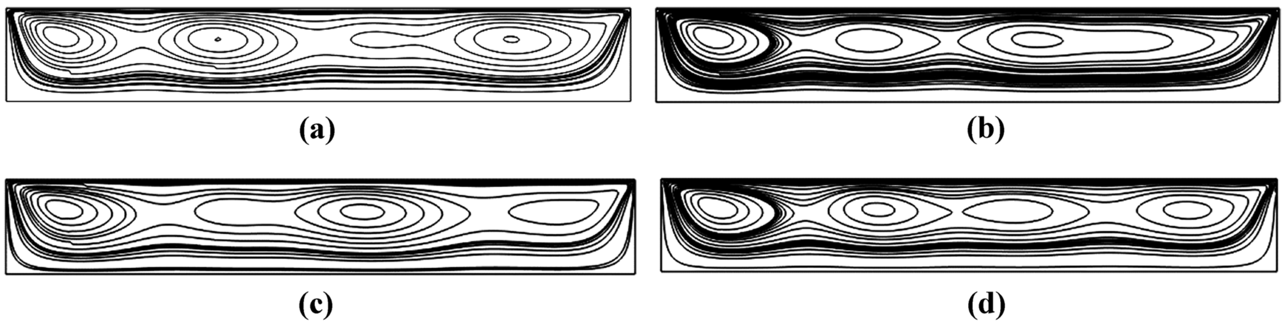

Fig. 2 Flow field evolution during one oscillatory period as $\Delta T = 2K$ and $\alpha_p = 0.01$ (**a**) $t = t_0$, (**b**) $t = t_0 + \tau/4$, (**c**) $t = t_0 + \tau/2$, (**d**) $t = t_0 + 3\tau/4$

Results and Discussions

When the temperature difference between the left and right walls is lower than the critical temperature difference, a steady thermocapillary convection will be formed in the cavity. The flow field consists of a larger convective cell and the flow at free surface from the hot end to the cold end. With the increase of temperature difference the thermocapillary flow will transits from steady to unsteady oscillatory flow. In particular, when the temperature difference is higher

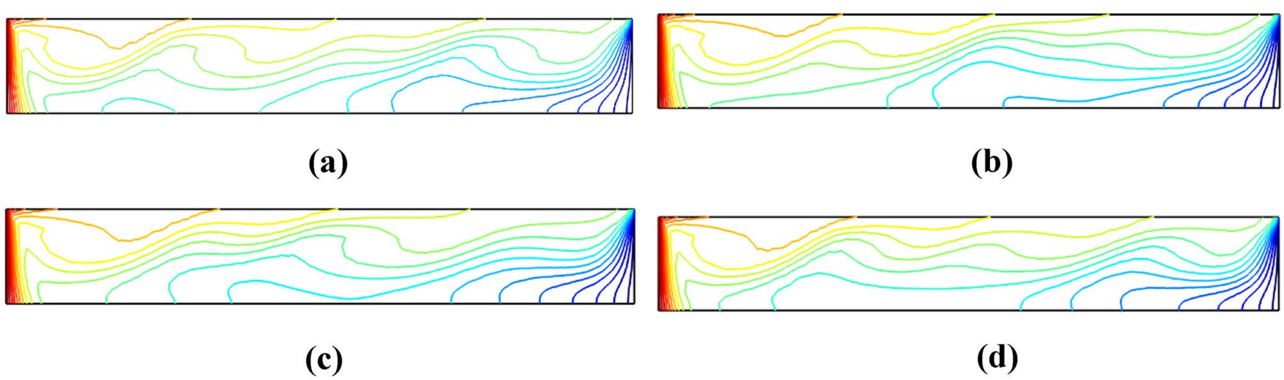

Fig. 3 Temperature field evolution during one oscillatory period as $\Delta T = 2K$ and $\alpha_p = 0.01$ (**a**) $t = t_0$, (**b**) $t = t_0 + \tau/4$, (**c**) $t = t_0 + \tau/2$, (**d**) $t = t_0 + 3\tau/4$

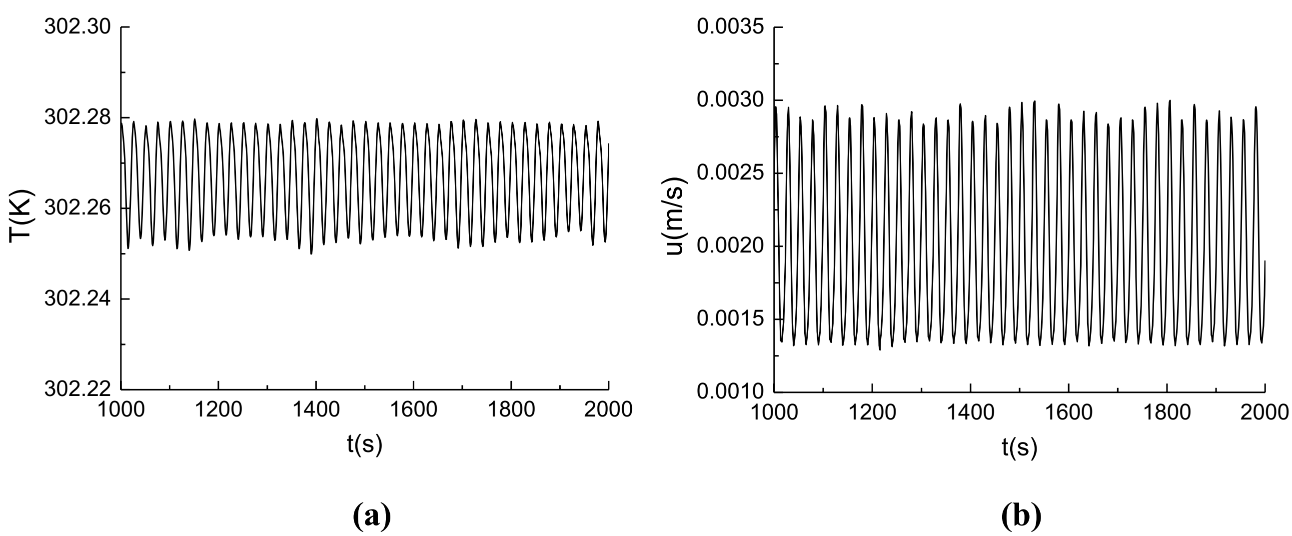

Fig. 4 Time history of temperature (**a**) and velocity (**b**) oscillation of monitoring point at free surface as $\Delta T = 2K$ and $\alpha_p = 0.02$

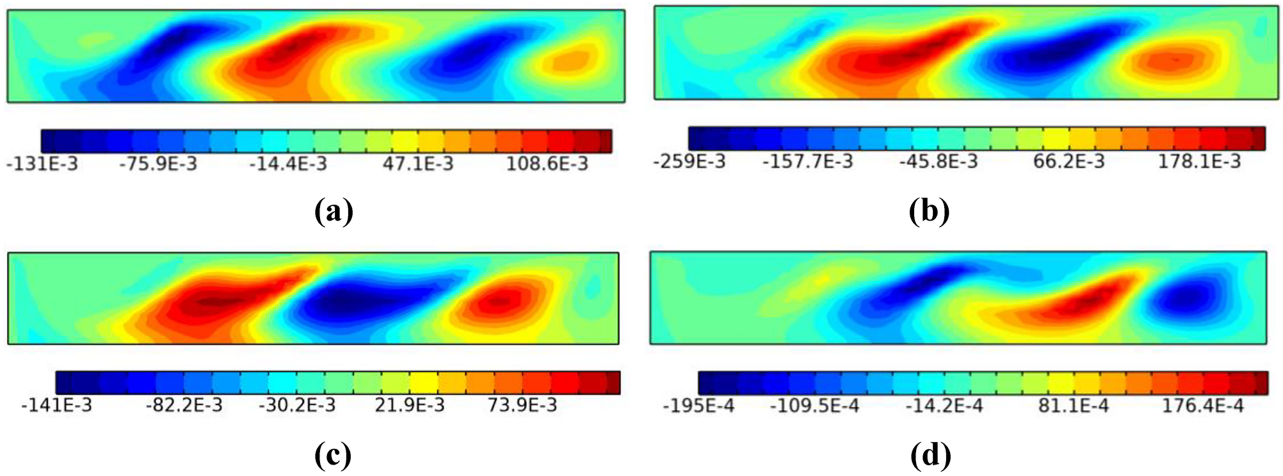

Fig. 5 Temperature fluctuation evolution during one oscillatory period as $\Delta T = 2K$ and $\alpha_p = 0.01$ (**a**) $t = t_0$, (**b**) $t = t_0 + \tau/4$, (**c**) $t = t_0 + \tau/2$, (**d**) $t = t_0 + 3\tau/4$

than the critical temperature difference (ΔT_{cri}), ΔT_{cri} is about 1.3 K in this two-dimentional cavity, the flow field disturbance first appears at the hot end. As the temperature difference increases to $\Delta T = 2K$, the disturbance vortex appears in the whole liquid layer. Figure 2 shows the flow field evolution during one oscillatory period as $\Delta T = 2K$ and $\alpha_p = 0.01$, from the figure we can see that, there is one cell located at the vicinity of the left wall and its shape and position remain unchanged. Meanwhile, at the central and right side regions the convective vortices keep periodic reciprocating migration in the cavity, and there are multiple flow patterns such as merging, splitting and migration of convective vortex. The corresponding temperature contours distribution is shown in Fig. 3. The isotherms also shows a periodic evolution, which is mainly reflected in the change of the dense area of the isotherms. The isotherm structure on the left remains basically stable, while the dense isotherm structure in the middle region gradually migrates to the right periodically. In order to further indicates the oscillatory characteristics of nanofluid thermocapillary convection, the history of temperature and velocity variation at monitoring point ($x = 10$ mm, $y = 3$ mm) is shown in Fig. 4. We can see that the temperaure and velocity value at monitoring point manifests a periodic oscillation.

In order to further demonstrate the disturbance characteristics of temperature field and velocity field, the fluctuations of temperature and velocity are defined as the difference between the instantaneous value and its time-averaged value, e.g., $\psi'(x, y, t) = \psi(x, y, t) - \psi_0(x, y)$, where $\psi'(x, y, t)$ is the temperature or velocity fluctuation and $\psi_0(x, z)$

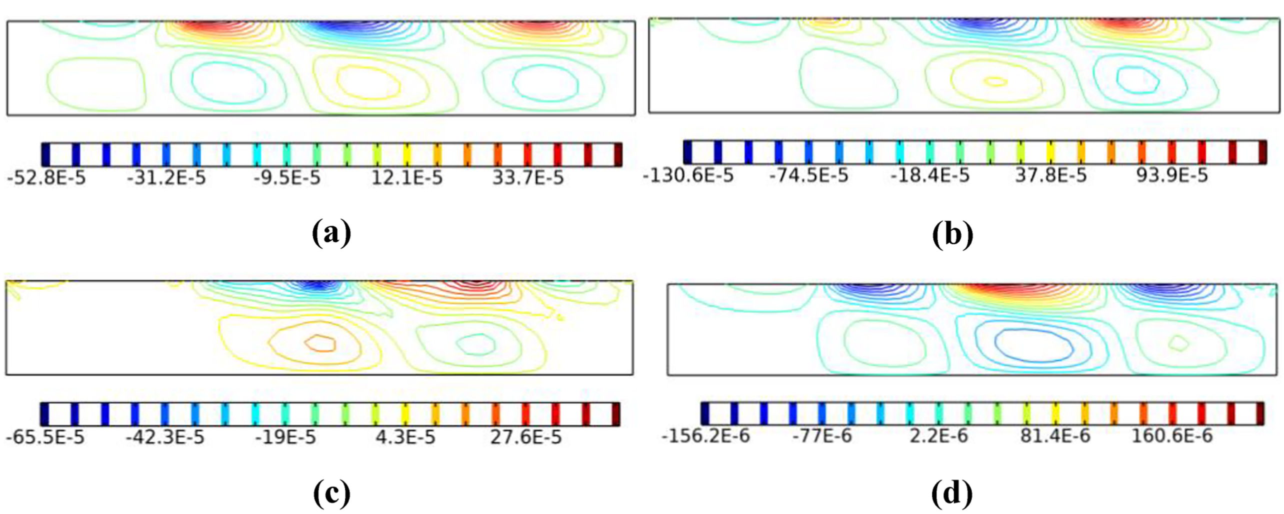

Fig. 6 Velocity fluctuation evolution during one oscillatory period as $\Delta T = 2K$ and $\alpha_p = 0.01$ (**a**) $t = t_0$, (**b**) $t = t_0 + \tau/4$, (**c**) $t = t_0 + \tau/2$, (**d**) $t = t_0 + 3\tau/4$

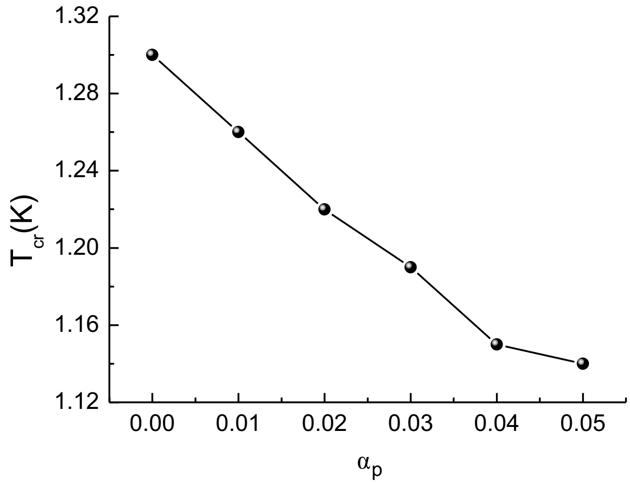

Fig. 7 Variation of critical temperature difference with nanoparticle volume fraction

$=\frac{1}{\tau'}\int_0^{\tau'}\varphi(x,y,t)dt$ is the time-averaged value, τ' is the time length much larger than the oscillation period (Li et al. 2016). Figure 5 gives the temperature fluctuation evolution during one oscillatory period as $\Delta T=2K$ and $\alpha_p=0.02$, it can be seen that temperature traveling wave appear in the whole liquid layer, and migrates from the right to the left side. The temperature fluctuation originates from the low temperature wall, and disappears at the vicinity of the high temperature wall. In the process of temperature wave propagation, the positive and negative deviations appear alternately, and the fluctuation range is variable. In particular, in the whole oscillation period the maximum fluctuation range is 0.45 K.

The evolution of velocity fluctuation during one oscillation period is shown in Fig. 6, it can be seen that the velocity fluctuation can be divided to two regions, namely, the upper free surface region and the lower fluid region. At the free surface region, the velocity fluctuation moves along free surface from the right to the left, and the positive and negative regions of velocity fluctuation appear alternately. Meanwhile, the evolution of velocity fluctuation at the lower fluid region also indicates the similar tendency, but its velocity fluctuation range is smaller. The fluctuation distribution indicates that the disturbance intensity at the free surface region is greater than that of the lower fluid region, this is due to the driving force of flow instability is located at the free surface. Moreover, it should be noted that the velocity fluctuation in the lower fluid region is opposite to that of the free surface region at the vertical direction, and the fluctuation range also changes periodically.

Figure 7 shows the variation of critical temperature difference of nanofluid thermocapillary convection with nanoparticle volume fraction, we can see that the critical temperature difference deceases gradually with nanoparticle volume fraction increasing, this means that nanofluid thermocapillary convection are more prone to instability than the base fluid. This tendency is caused by the change of nanofluid thermophysical properties due to the increase of nanoparticles, namely the addition of nanoparticle leads to the increase of thermal conductivity and dynamic viscosity, then thermal diffusivity increases but the momentum diffusivity decreases, so the nanofluid thermocapillary convection becomes more unstable.

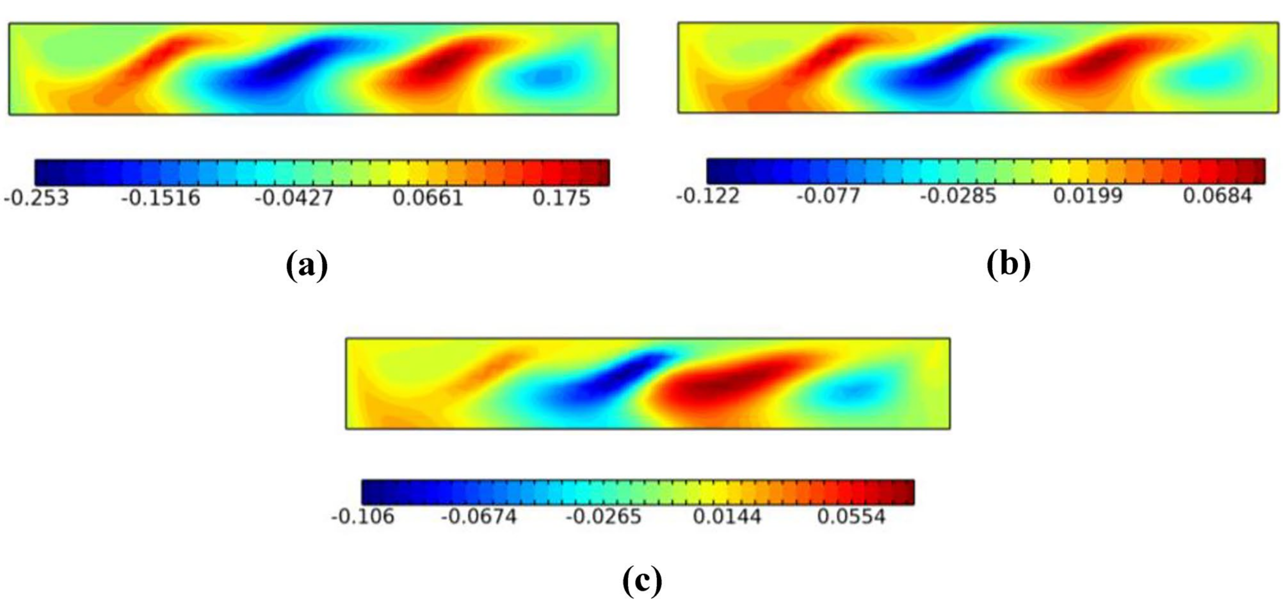

Fig. 8 Temperature fluctuation distribution under different nanoparticles volume fractions as $\Delta T=2K$ (**a**) $\alpha_p=0.01$, (**b**) $\alpha_p=0.03$, (**c**) $\alpha_p=0.05$

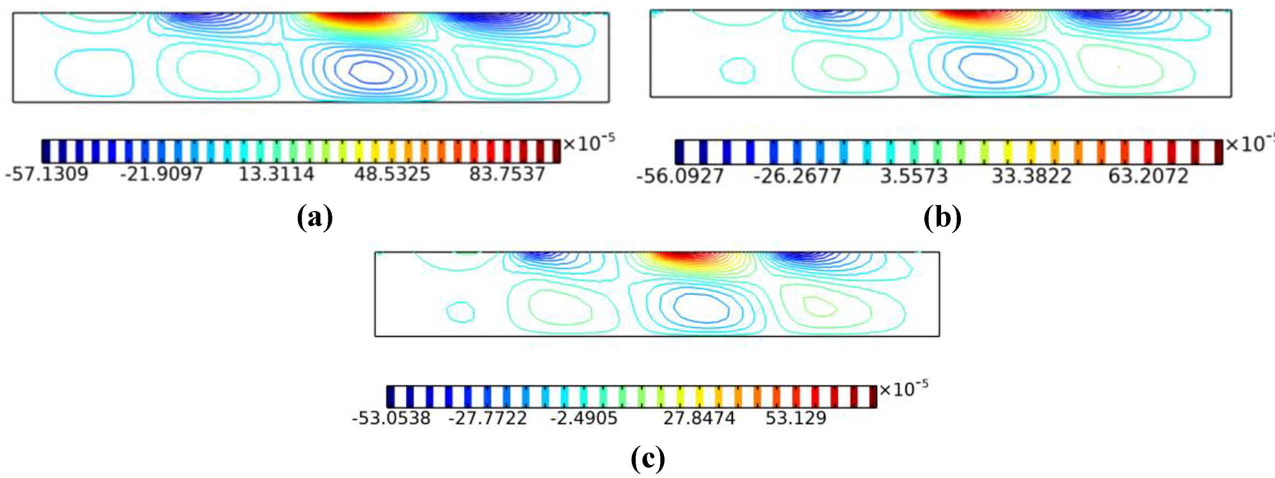

Fig. 9 Velocity fluctuation distribution under different nanoparticles volume fractions as $\Delta T=2K$ (**a**) $\alpha_p=0.01$, (**b**) $\alpha_p=0.03$, (**c**) $\alpha_p=0.05$

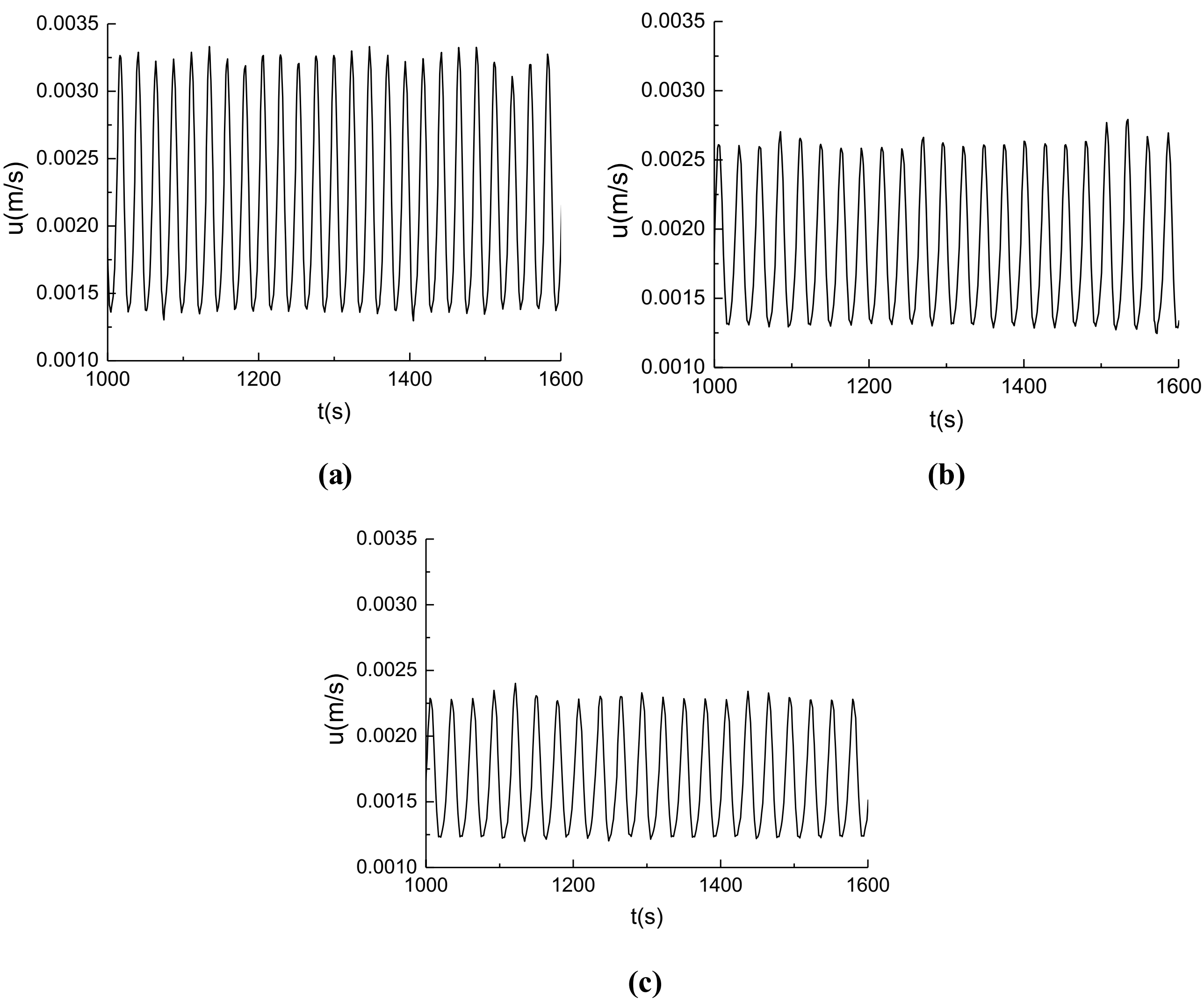

Fig. 10 Time history of velocity oscillation at monitoring point under different nanoparticle concentration as $\Delta T=2K$ (**a**) $\alpha_p=0.01$, (**b**) $\alpha_p=0.03$, (**c**) $\alpha_p=0.05$

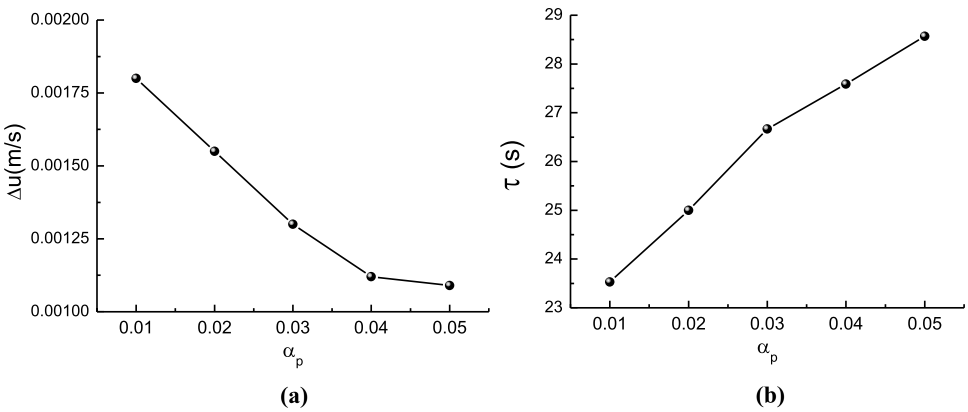

Fig. 11 Variation of average velocity oscillatory amplitude (**a**) and period (**b**) at monitoring point with nanoparticle volume fraction as $\Delta T = 2K$

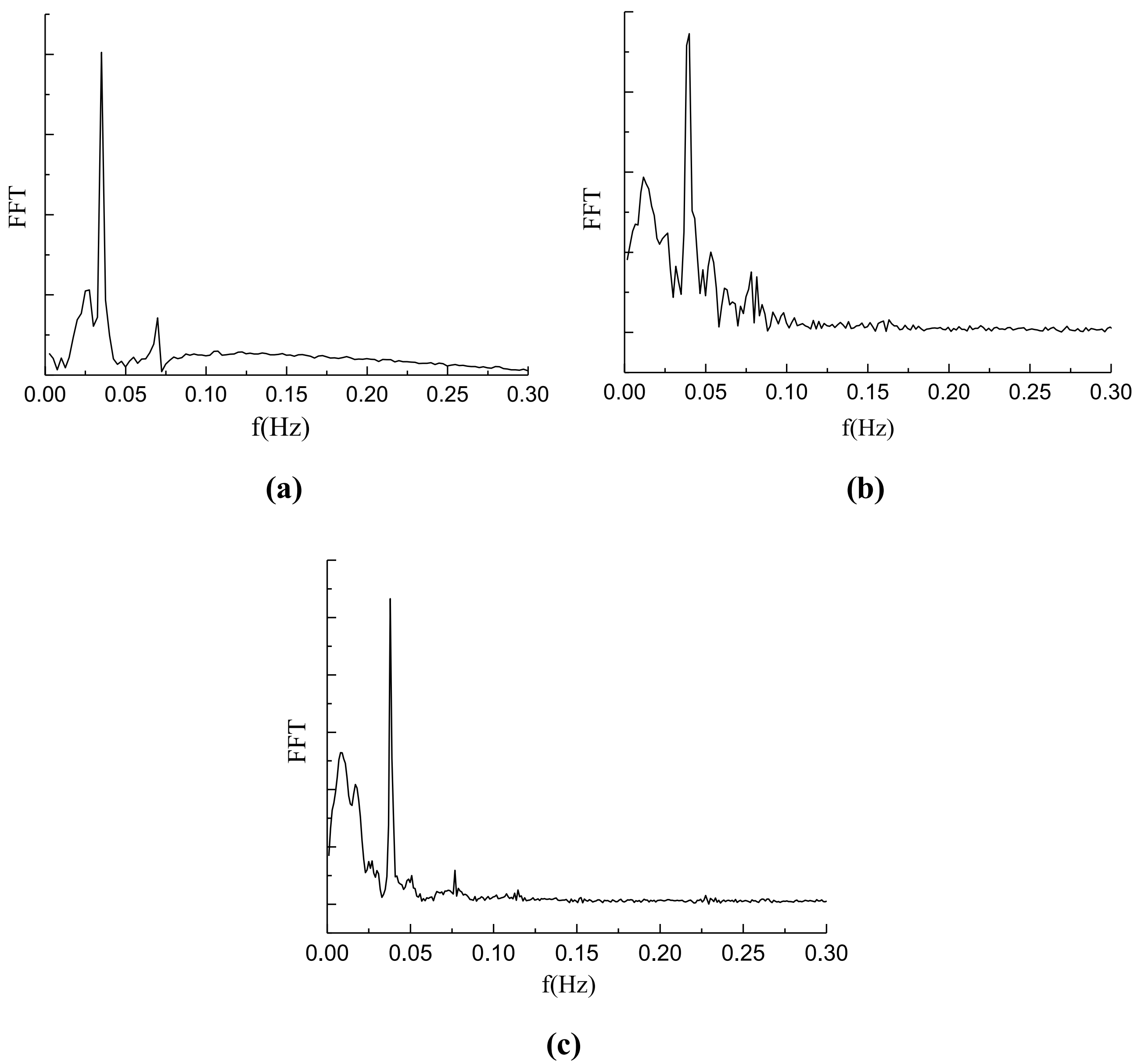

Fig. 12 Power spectra of the surface velocity flctuations with different nanoparticles volume fractions as $\Delta T = 2K$ (**a**) $\alpha_p = 0.01$, (**b**) α_p 0.03, (**c**) $\alpha_p = 0.05$

Figures 8 give temperature fluctuation distribution under different nanoparticles volume fractions as ΔT = 2K. According to Fig. 5, the temperature fluctuation is variable durring one oscillatory period, so we give the temperature fluctuation distribution when the temperature value of the monitoring point is at the peak. It can be seen that, under different nanoparticles volume fractions the temperature fluctuation distibution behaves the same mode, and there are only slight differences in the structure of temperature waves. With nanoparticle volume fraction increasing the range of temperature fluctuation decreases gradually, this is due to the heat transfer is enhanced by the addtion of nanoparticle. The corresponding velocity fluctuation under different nanoparticles volume fractions is given in Fig. 9, similary to that of temperature deviation, the range of velocity fluctuation also decreases gradually as nanoparticle volume fraction increases.

Figure 10 gives the time history of velocity oscillation at monitoring point (x = 10 mm, y = 3 mm) under different nanoparticle concentrations as ΔT = 2K. It can be seen that under different nanoparticle vonlume fractions the velocity evolution history at monitoring point demonstrates the similar oscillation characteristics, however, the range of velocity oscillation and the oscillation period is different. In particularly, the maximum velocity decreases from 0.00325 m/s at $\alpha_p = 0.01$ to 0.0023 m/s at $\alpha_p = 0.05$, at the same time the oscillation period also is increased. In order to show the detailed change of oscillation characteristics, Fig. 11 presents the variation of average velocity oscillatory amplitude and period at monitoring point with nanoparticle volume fraction as ΔT = 2K. With nanoparticle volume fraction increasing the velocity oscillatory amplitude decreases, and the decrease rate is reduced grdually. Meanwhile, the oscillatory period increases almost linearly with nanoparticle volume fraction. This change tendency shows that the oscillation characteristics of thermocapillary convection can be adjusted by the concentration of nanoparticles.

Furthermore, the spectrum analysis of velocity history at monitoring point under different nanoparticle volume fraction is shown in Fig. 12, for all the cases with different nanoparticles volume fractions the flow field oscillation just has one dominant oscillation frequency and the frequency is about 0.046 Hz, but with nanoparticles volume fraction increasing the second fundamental frequency begins to appear and strengthens gradually.

Conclusions

In this paper, the numerical investigation of moderate Prandtl number nanofluid thermocapillary convection instability in a two-dimensional rectangular cavity is carried out, and the effect of nanoparticle volume fraction on thermocapillary convection is analyzed. The conclusions are drawn as follows:

1) The critical temperature difference deceases gradually with nanoparticle volume fraction increasing, and the nanofluid thermocapillary convection are less stable than the base fluid.
2) With nanoparticle volume fraction increasing, the velocity oscillatory amplitude decreases and the oscillatory period almost increases linearly.
3) Nanofluid oscillatory thermocapillary convection has one dominant oscillation frequency and the frequency is about 0.046 Hz, but with nanoparticles volume fraction increasing the second fundamental frequency strengthens gradually.

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Data Availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Conflict of Interest We declare that we have no financial and personal relationships with other people or organizations that can inappropriately influence our work, there is no professional or other personal interest of any nature or kind in any product, service and/or company that could be construed as influencing the position presented in, or the review of, the manuscript entitled, "Moderate Prandtl number nanofluid thermocapillary convection instability in rectangular cavity".

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