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Numerical Study of Nonlinear Structures of Locally Excited Marangoni Convection in the Long-Wave Approximation

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Abstract

We investigate stationary and non-stationary solutions of nonlinear equations of the long-wave approximation for the Marangoni convection caused by a localized source of heat or a surface active impurity (surfactant) in a thin horizontal layer of a viscous incompressible fluid with a free surface. The distribution of heat or concentration flux is determined by the uniform vertical gradient of temperature or impurity concentration, distorted by the imposition of a slightly inhomogeneous heating or of surfactant, localized in the horizontal plane. The lower boundary of the layer is considered thermally insulated or impermeable, whereas the upper boundary is free and deformable. The equations obtained in the long-wave approximation are formulated in terms of the amplitudes of the temperature distribution or impurity concentration, deformation of the surface, and vorticity. For a simplification of the problem, a sequence of nonlinear equations is obtained, which in the simplest form leads to a nonlinear Schrödinger equation with a localized potential. The basic state of the system, its dependence on the parameters and stability are investigated. For stationary solutions localized in the region of the surface tension inhomogeneity, domains of parameters corresponding to different spatial patterns are delineated.

Keywords Marangoni convection · Long-wave approximation · Amplitude equations · Nonlinear localized structures

Introduction

A source of inhomogeneity in temperature or surfactant concentration, positioned near the liquid-gas interface, changes the surface tension and can influence heat-mass transfer in the adjacent area, affecting further the entire volume of fluid. By means of the Marangoni effect, it can generate the intensive convective flow (Nepomnyashchy et al. 2002).

Studies of the Marangoni convection caused by inhomogeneities of surface tension, localized near the liquid interfaces, are of special interest because of numerous technological applications (processes in special metallurgy, material science, inhomogeneous chemical reactions, microfluidic devices etc.) and of the fundamental role played by processes on the phase boundary in understanding new mechanisms of the instability of the ground state of a hydrodynamic system. In comparison with the case of uniform ambient conditions, such flows are less studied, hence various phenomena, observed experimentally, are still lacking rigorous explanations.

In the most general way, the problem may be formulated as investigation of convection in the shallow horizontal liquid layer where the inhomogeneities of both density and surface tension are caused by localized sources of either thermal or concentration nature. We assume either a sufficiently thin layer or the microgravity conditions, so that the influence of inhomogeneity of surface tension (Marangoni convection) would be predominant. Studies of the Marangoni convection in shallow horizontal liquid layers with non-uniform distributions of surface tension, caused either by localized sources of temperature or by concentration inhomogeneities, are pursued for many years.

For the case of a surfactant source, some remarkable effects were observed experimentally. In particular, for the water-alcohol solution that contained the source of the

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surfactant admixture, the sequence of flow instabilities was reported, leading to the onset of the multi-petal flow pattern with even number of petals, dependent on the source intensity (Pshenichnikov and Yazenko 1974). Those experiments found a further development in Mizev (2005), where the essential influence of the adsorption of surface-active admixture on the structure and stability of concentration-capillary flow was established. Among the recent achievements in this problem is the disclosure in precise experiments (Mizev et al. 2013) of the substantial influence of addition of surfactant to the liquid surface: its amount (not controlled in previous experiments) predetermines the main features of the flow patterns, including the size of the annular domain of vortical flow, and the number of azimuthal vortices (petals) therein.

In experiments, the thermocapillary effect can be produced by a solid heater, by the low intensity laser or by the other source of radiation that influences the upper boundary of the horizontal fluid layer and causes the non-uniform temperature distribution, shaped as a hot spot in the vicinity of the interface. Among the results concerning the localized heat sources, it is worth to mention the experiments demonstrating similar multi-petal patterns caused by the influence of the thermal inhomogeneities due to the heat source placed on the bottom (Ezersky et al. 1993), and the experiments (Mizyov et al. 2000; Karlov et al. 2005), in which the localized heat source has been generated by a laser or incoherent radiation.

In these experiments, the fluid flow near the hot spot may vary in structure and have variously shaped menisci depending on the intensity of radiation, the thickness of the layer, and the form of heat inhomogeneity. Similar and even more intricate formations were observed experimentally, when the localized solid source of heat was either placed on the bottom of the cavity, or immersed in the liquid at the certain depth. In that case the meniscus oscillations followed by concentric and spiral waves on the free surface that were observed in the laboratory experiments (Mizyov et al. 2000), still have no theoretical explanation.

For other kinds of fluid flows, the substantial influence of local heating upon the thermocapillary driven change of surface deformation and the resulting instabilities was studied experimentally for shear driven horizontal thin films (Kabova et al. 2009) and for thin falling films on vertical surfaces (Kabov et al. 2002).

Important theoretical studies of the problem include analytical solutions derived respectively for the point and extended heat sources (Bratukhin and Maurin 1982; Bratukhin and Makarov 2005), and the simplified theoretical description of the aforementioned oscillatory instability in one-dimensional formulation (Mizyov et al. 2000). The article (Boeck and Karcher 2003) contains results of computer simulation of the problem in 3D in the assumption of non-deformable surface, in particular, the steady patterns with the symmetry of fourth order were obtained.

3D calculations were performed also for the case of a fluid layer with a non-deformable free surface in a cylindrical container, locally heated from below at the center of the bottom (Navarro et al. 2007). It has been shown that the basic state may bifurcate to different patterns, depending on the shape and parameters of the heating function. Various kinds of instabilities, both of global and local character, were reported to result in targets and spiral waves.

Different forms of long-wave approximations have been developed for this class of problems, including integral boundary layer approximation for thin locally heated falling liquid films (Kalliadasis et al. 2003), temperature amplitude equation for thermal convection in the locally heated thin layer with rigid boundaries (Lyubimov, Tcherepanov,1991) and the model with amplitude equations, governing temperature, vorticity and surface deformation for thermocapillary convection in a uniformly heated two-layer system (Golovin et al. 1995).

Theoretical and numerical treatment of the problem of solutocapillary convection with inhomogeneous concentration distribution was implemented by Birikh et al. (2009), who investigated numerically the concentration convection in an isothermal liquid near a drop (or an air bubble) clamped between the vertical walls of a horizontal channel; they used models both with and without account of the surface phase at the drop–liquid interface formed by adsorption/desorption process. This approach permits to take into account interactions between the buoyancy and the Marangoni convective flows leading to the auto-oscillatory regime observed in experiments. To the knowledge of the author, numerical investigations of the problem for localized inhomogeneous distribution of the impurity at the boundary are practically absent. A similar problem for the annular pool subjected to a constant radial solutal gradient, in the full 3D formulation for non-deformable surfaces is dealt with in the recent paper (Chen et al. 2016), where the critical solutal capillary Reynolds (Marangoni) numbers of transition from steady axisymmetric flow to oscillatory axisymmetric or 3D flow have been determined.

Long-wave approximation to the solutocapillary problem is applied to the case of homogeneous distribution of impurity concentration at the boundaries by Mikishev and Nepomnyashchy (2011). In this work the governing amplitude equations are obtained for impurity concentration in the bulk flow, surface deformation and the specific variable for solutocapillary convection – the impurity concentration on the boundary.

The present study offers the general mathematical formulation of problem of Marangoni convection caused by localized surface tension inhomogeneity, both of thermo- and solutocapillary origin; the long–wave approximation

of the problem is accepted for the case of thin layer, and some further possible simplifications are analyzed. This theoretical approach continues the study of thermocapillary convection at localized heating (Wertgeim and Myznikova 2002), based on the model that generalizes the long-wave description of the uniformly heated two-layer system (Golovin et al. 1995) to the case of inhomogeneous heating. Basing on this model, it becomes possible to explain the effects of change of the surface configurations, including the concave, convex and concavo-convex types of meniscus, observed in the laboratory experiments on localized laser heating under the surface of horizontal liquid layer (Karlov et al. 2005).

Analysis of the above mentioned results allows us to conclude that theoretical and numerical studies of experimentally observed complex behavior of convective systems with interfaces should in general be based on the results of calculations in the complete three-dimensional formulation, which has so far been realized only for the limiting cases of non-deformed interfaces or by neglecting thermal and/or concentration perturbations. A promising alternative approach to the problem has been proposed and implemented, based on amplitude equations of long-wave approximation, applicable for the considered case of a thin layer. This approach makes it possible to reduce the solution of the problem in the complete three-dimensional formulation to a two-dimensional one. Strict validity of this reduction holds only for a range of the parameters of the problem close to critical value for onset of instability of the ground state. Nevertheless, this approach has rich possibilities for studying various types of boundary conditions, forms of inhomogeneity of heat flux or impurity distribution etc., and allows one to advance into the region of existence of developed nonlinear regimes, and, with minor modification, to treat also the time-periodic variants of localized heat flux (Wertgeim et al., 2013). Another interesting direction of studies is related to the processes of adsorption and desorption on the interface "liquid-gas". Simulation of these phenomena requires improved mathematical models due to the introduction of the additional equation for the propagation of adsorbate at the liquid surface (Bratukhin and Makarov 2005; Birikh et al. 2009).

It was established (Wertgeim and Myznikova 2002; Karlov et al. 2005) that equations describing the development of long-wave disturbances caused by heat flux inhomogeneity in the form of a step function display only a monotonic instability of the main flow. For a more general forms of inhomogeneity of the heat flux, remarkable results have been obtained (Kumachkov and Wertgeim 2009) on the presence of narrow parameter regions corresponding to abrupt changes in the form of the stationary solution, in particular, the transition from the hump to the depression

for deformation of the surface. This effect was observed in experiments on localized heating of the near-surface region by laser or incoherent radiation.

The aim of the present work is to consider these phenomena with more details, to elucidate the reasons for the appearance of the selected values of the parameters corresponding to abrupt changes in the form of stationary solutions, to study their stability and nonlinear evolution.

Formulation of the Problem

A mathematical description of the above described processes is based on the three-dimensional boundary-value problem for the non-linear system of equations of convective heat or mass transfer and deformation of the surface of the viscous incompressible fluid.

Consider a thin infinite horizontal layer of viscous incompressible fluid. The lower boundary $z = 0$ is assumed to be solid and either heat-insulated or impermeable; the half-space above the upper free boundary $z = L + h(x, y, t)$ is assumed to be the air, not dissolvable in the liquid.

Assumption of the small thickness of the layer implies that the influence of the Marangoni force is predominant, making it possible to disregard the effect of the buoyancy, and to write down the system of governing equations in terms of the horizontal components $\vec{u}(x, y, z, t)$ and the vertical component $w(x, y, z, t)$ of velocity, and either temperature $T(x, y, z, t)$ or surfactant concentration $C(x, y, z, t)$ (below we will use the common notation $S(x, y, z, t)$ for any of last two variables, changing the surface tension according to the expression $\sigma = \sigma_0 - \sigma_s S$). In dimensionless variables the system of governing equations reads

$$\frac{1}{d}\left\{\partial_t \vec{u} + (\vec{u}\nabla)\vec{u} + w\vec{u}'\right\} = -\nabla p + \Delta\vec{u} + \vec{u}'', \quad (1)$$

$$\frac{1}{d}\left\{\partial_t w + \vec{u}\nabla w + ww'\right\} = -p' + \Delta w + w'' - G, \quad (2)$$

$$\nabla \cdot \vec{u} + w' = 0, \quad (3)$$

$$\partial_t S + \vec{u}\nabla S + wS' = \Delta S + S'' + \mu(\Delta q + q_z'') \quad (4)$$

The primes denotes derivatives with respect to the vertical coordinate z.

On the horizontal boundaries of the layer the heterogeneity of temperature or surfactant concentration is described using function $Q(x, y, z) = q(x, y) \cdot q_z(z)$, taken at the lower boundary $z = 0$ and upper deformable boundary $z_h = 1 + h(x, y, t)$ respectively. These two values are inhomogeneous part of heat flux in the thermocapillary case and the surfactant flow rate in solutocapillary situation. The

dependence of Q on z was introduced to reflect the presence in the experiments of a localized heat source below the liquid surface caused either by a laser (Karlov et al. 2005) or by incoherent (Mizev 2004) radiation. In a complete three-dimensional formulation (1)–(4), this leads to the appearance in the right hand side of Eq. 4 of the term with internal heat source $\mu \Delta Q(x, y, z)$ due to absorption of light, where the coefficient μ is determined by the ability of the medium to absorb light (Gershuni et al. 1989). For the solutocapillary case, the situation with submerged source of surfactant is more hard to realize experimentally, so further it will be assumed that in this case $q_{z.} = const = 1, \mu = 0$. Accordingly, the boundary conditions for system (1)–(4) are

$$z = 0 : \vec{u} = w = 0; \; S' = -1 + q(x, y) \cdot q_z(0);$$
$$z = 1 + h(x, y) : h_t + \vec{u} \nabla h = w; \quad (5)$$
$$S' = \nabla h \nabla S - 1 + q(x, y) \cdot q_z(1); \; q'_z(1) \equiv \zeta.$$

In addition, on the interface $z = z_h = 1 + h(x, y, t)$ the balance of normal and tangential components of the momentum flux density $\Pi_{ik} = -p\delta_{ik} + (V_{i,k} + V_{k,i})$ is ensured by the following relationships (in assumption of no adsorption of surfactant on the surface):

$$\Pi_{nn} = \nabla \left(\frac{\nabla h}{\sqrt{1 + (\nabla h)^2}} \right) (Ca - Ma\, S), \quad (6)$$

$$\Pi_{nt_i} = Ma \left(\frac{1}{\sqrt{1 + (\partial_i h)^2}} \right) (\partial_i S - S' \partial_i h) \quad (7)$$

The model described by Eqs. 1–7 contains the following dimensionless parameters: the Marangoni number $Ma = \sigma_S \tilde{Q} L^3 / (\eta \chi)$; the Prandtl or Schmidt number d ($d = Pr = \nu/\chi$) for thermocapillary case and $d = Sc = \nu/D$ for solutocapillary case); the Galileo number $G = gL^3 / (\nu \chi)$ and the capillary number $Ca = \sigma L / (\eta \chi)$. The symbols $\eta, \nu, \chi, D, \sigma$ denote the coefficients of the dynamic viscosity, kinematic viscosity, thermal diffusivity and surface tension, respectively; $\tilde{Q}$ stands for either the dimensional power of the heater or consumption of the surfactant, and L for the depth of the layer. The parameter ζ in Eq. 2 will appear later in equations of long-wave approximation ("Formulation of the Problem") and characterizes the vertical inhomogeneity of heat or surfactant source. Value of $\zeta = 0$ corresponds to $q_z(z) = const$, ζ is negative for the case of the source under the surface, and a change in this coefficient can simulate a change in the depth of immersion of a heat or concentration source.

In the solutocapillary case, when $S \equiv C$, only the simplest case of soluble surfactant with absent surface concentration is considered here. This is actually equivalent to the thermocapillary case, with a replacement of the Prandtl number by the Schmidt number. Possible modifications to be investigated elsewhere include account of finite distribution of surface concentration $\Gamma(x, y, z_h)$ determined by processes of diffusion, convective transport, and adsorption/desorption on the surface. The coefficient of surface tension on the interface in this case is set as $\sigma = \sigma_0 - \sigma_c C - \sigma_\Gamma \Gamma$. The problem reformulation requires an additional equation for the surface concentration of the surfactant $\Gamma(x, y, z_h)$, and the change of boundary conditions on deformable surface (5) and (6), transforming them into the equation for the velocity on the surface. In the simplified case of a non-deformable surface the corresponding changes are as follows (Birikh et al. (2009)):

$$\partial_t \Gamma + \nabla(\vec{u}\, \Gamma) = Sc_s^{-1} \Delta \Gamma + Sc^{-1}(K_a \cdot C - K_d \cdot \Gamma) \quad (8)$$

$$\Gamma \partial_t \vec{u} + \Gamma(\vec{u}\nabla)\vec{u} = \Pi_{zx} - Ma(\nabla C - Sc^{-1}\nabla \Gamma) \quad (9)$$

$$C' = -1 + q(x, y) \cdot q_z(1) + K_a \cdot C - K_d \cdot \Gamma; \quad (10)$$

Here several new non-dimensional parameters appear: Sc_s, K_a, K_d being the surface Schmidt number, characterizing diffusion of Γ on the surface, and coefficients of adsorption and desorption of the surfactant respectively.

For the case of no adsorption and desorption ($\Gamma = K_a = K_d = 0$) the boundary conditions (8)–(10) coincides with (5)–(7) for non-deformable surface. The account of both surface deformation and adsorption/desorption processes would require more complicated equations and boundary conditions than (8)–(10) (cf. Mikishev and Nepomnyashchy 2011).

The Long-Wave Approximation

Separation of characteristic horizontal and vertical scales of the formulated problem (the characteristic horizontal scale of surface tension inhomogeneity exceeds noticeably the thickness of the liquid layer) allows sufficient simplification in the mathematical formulation of problem, without detriment to its physical essence.

Namely, we could apply the long-wave approximation slightly beyond the threshold of onset of thermocapillary or solutocapillary convection $Ma_{cr} = 48$ (this threshold corresponds to the long-wave instability, described by Golovin et al. (1995) for the limiting case of a uniformly heated layer with a thermally insulated bottom). In accordance with the perturbation technique, the expansions are performed into the powers of the small parameter ε, characterizing the ratio of vertical and horizontal scales: $\varepsilon^2 \equiv (\partial f / \partial x) / (\partial f / \partial z)$. The following asymptotic expansions are obtained for the velocity, temperature or

surfactant concentration, pressure, surface deformation and surface concentration of the surfactant:

$$\vec{u} = \sqrt{\varepsilon}(\vec{u}_0 + \varepsilon \vec{u}_1 + \varepsilon^2 \vec{u}_2 + ...);$$
$$w = \varepsilon(w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + ...);$$
$$h = \varepsilon(H_0 + \varepsilon H_1 + ...);$$
$$p = \varepsilon^{-1} P_{-1} + P_0 + \varepsilon P_1 + ...$$
$$S = S_0 + \varepsilon S_1 + \varepsilon^2 S_2 + ...; \tag{11}$$

$$\Gamma = \Gamma_0 + \varepsilon \Gamma_1 + ...$$

We treat the heat or mass inhomogeneity as weak, of the first order with respect to ε, as it was done in the studies of thermogravitational convection from inhomogeneous heat source (Lyubimov and Tcherepanov 1991). The following rescaling is adopted:

$$(x, y) \rightarrow \sqrt{\varepsilon}(x, y); \quad t \rightarrow \varepsilon^2 t;$$

Considering the low orders (-1; 0) in expansions (8), the following relations were obtained for 2D amplitudes of flow characteristics (Golovin et al. 1995; Wertgeim and Myznikova 2002):

$$P_{-1} = G(1 - z); \ P_0 = GH - Ca\Delta H; \ S_0 = -z + \Phi;$$
$$\vec{u}_0 = 12 f'(z)\nabla\Phi; \ w_0 = -12 f(z)\Delta\Phi. \tag{12}$$

After the expansion until the second order, the mathematical model acquires the form of the system of nonlinear differential equations for two-dimensional amplitudes of the functions $\Phi(x, y)$, $\Psi(x, y)$, and H(x, y), (H $\equiv H_0$)characterizing respectively the deviation of the field S from the equilibrium distribution with a vertical gradient, the vorticity, and the free surface deformation:

$$\partial_t \Phi + \nabla\Phi \ \nabla \times (\vec{e}_z \Psi) + a_1 \nabla^4 \Phi - \nabla^2 H - a_2 \nabla \left(|\nabla\Phi|^2 \nabla\Phi \right)$$
$$+ a_3 \nabla \left(\nabla^2 \Phi \ \nabla\Phi \right) + a_4 \nabla^2 |\nabla\Phi|^2 \ + a_5 \nabla(H\nabla\Phi)$$
$$- \nabla(q\nabla\Phi) + a_6 \nabla^2 q + \zeta q H = 0 . \tag{13}$$

$$\vec{e}_z \nabla^2 \Psi = b_1 \nabla(\nabla^2\Phi) \times \nabla\Phi - b_2 \nabla H \times \nabla\Phi; \tag{14}$$

$$\nabla^4 H - c\nabla^2 H = \delta\nabla^2\Phi. \tag{15}$$

In Eqs. 12–15 the following notations are used:

$$f(z) \equiv z^2 - z^3; \quad \vec{e}_z = (0, 0, 1);$$
$$a_1 = \tfrac{1}{15}, \ a_2 = \tfrac{48}{35}, \ a_3 = \left(\tfrac{1}{10} + \tfrac{1}{5d}\right), \ a_4 = \left(\tfrac{3}{5} + \tfrac{1}{10d}\right),$$
$$a_5 = 2, \ a_6 = 0.5, \ b_1 = \tfrac{312}{3d}, \ b_2 = 24.$$

In these equations, additional rescaling, $G \rightarrow \varepsilon G; Ca \rightarrow \varepsilon^2 Ca$ is adopted, and only the parameters connected with the rescaled inverse capillary number Ca and Galileo number G, $c = 72/Ca$, $\delta = G/Ca$ remain. The values $c = \delta = 0$ correspond to the case of a non-deformable

upper surface. The system (13)–(15) generalizes the set of equations obtained for the long-wave Marangoni convection in the uniformly heated layer (Golovin et al. 1995),the last three terms in Eq. 9 describe the influence of the inhomogeneity of heat flux. In the case of solutocapillary convection, the account of adsorption-desorption processes on the interface (5)–(7) yields additional equations for Γ_0, Γ_1, and corresponding changes in Eqs. 13–15.

Thus, the system of nonlinear amplitude equations (13)–(15) describes the evolution of long-wave disturbances of the temperature or surfactant concentration field, the fluid velocity, and the deviation of free surface from the plane, that develop in the horizontal layer as a result of the weak non-homogeneity of the surface tension due to heat or surfactant action. In contrast to the similar system, described in Golovin et al. (1995) for the uniformly heated layer, Eq. 9 contains additional terms, two of them reflecting the spatial inhomogeneity in the horizontal direction, and the third one, the last term of Eq. 9, is generated by the thermal (or concentration) source inhomogeneity across the vertical coordinate.

Variants of Localized Surface Tension Inhomogeneity

The inhomogeneous surface tension is supposed to be localized in the horizontal plane. Two variants of its horizontal configuration, described by the function $q \ (x, y)$, were considered, both depending from single spatial variable ξ, whose meaning depends on the problem symmetry: namely, $q = q(\xi)$, where $\xi \equiv x$ for the plane source of inhomogeneity and $\xi \equiv r$ for an axisymmetric source. As a function describing surface tension inhomogeneity, the smooth function of one of the following types is chosen:

$$\text{I.} \quad q(\xi) = \left(\beta^2 \sinh^2(\beta\xi) - \alpha^2\right) \Big/ \cosh^2(\beta\xi), \tag{16}$$

$$\text{II.} \quad q(\xi) = -A + B\tanh((\xi - R)\big/\rho), \tag{17}$$
where
$$A = \left(\alpha^2 - \beta^2 \tanh(R\big/\rho)\right) \Big/ (1 + \tanh(R\big/\rho)) ;$$
$$B = \beta^2 + A.$$

The parameters in the definition of $q(\xi)$ characterize, respectively, the deviation of the heat or mass flux from its threshold value at the onset of thermo- or soluto-capillary convection both inside (α) and outside (β) the area of surface tension inhomogeneity; the characteristic size (R) of the inhomogeneity; and the width (ρ) of the interval where the smoothing is performed of the sharp boundary between the hot spot and the remaining part of the plate.

The choice of function $q(\xi)$ in the case I owes to the fact that solutions of Eqs. 13–15 with this kind of heat flux

inhomogeneity in the limit case of underformable surface can be compared with exact stationary solution obtained in (Lyubimov, Tcherepanov, 1991), and can be used for testing of numerical methods. For the case II the choice is connected with possibility of comparison to the results of the linear analysis (Wertgeim and Myznikova 2002; Karlov et al. 2005), where the stepwise heat inhomogeneity was accepted. The stepwise function is the limit case of the dependence (17) at $\rho \to 0$.

Steady Solutions: 1D Problem and its Simplifications. Methods of Solution

Further consideration concerns only the case of inhomogeneity of surface tension due to the horizontal heat flux inhomogeneity $q = q(\xi)$, which physically corresponds to a plane hot bar (in 1D plane case) or to an axially symmetrical hot spot. These results can also be applied to the case of admixture addition to the surface, spread to the bulk of liquid without account of surface concentration of a surfactant ($\Gamma = 0$), for which the problem formulation is equivalent to the case of a localized heat source.

The localized steady solution of Eqs. 13–15 is assumed to have the same symmetry that the inhomogeneity of the heating (this is not rigorously proved, but 2D numerical simulations have confirmed this conjecture). We shall use the subscript "0" for this steady solution (it is easy to see that in the cases under consideration the vorticity field is absent for steady state due to the suggested symmetry):

$$\Phi_0 = \Phi_0(\xi), \quad H_0 = H_0(\xi), \Psi_0 = 0. \tag{18}$$

The governing equations for the basic state (14) are reduced from Eqs. 13–15 to the following system:

$$a_1\nabla^4\Phi_0 - \nabla^2 H_0 - a_2\nabla\left(|\nabla\Phi_0|^2\nabla\Phi_0\right) + \\ a_3\nabla\left(\nabla^2\Phi_0\nabla\Phi_0\right) + a_4\nabla^2|\nabla\Phi_0|^2 + a_5\nabla\left(H_0\nabla\Phi_0\right) \\ + \nabla\left(q\nabla\Phi_0\right) + a_6\nabla^2 q + \zeta q H_0 = 0 \tag{19}$$

$$\nabla^4 H_0 - c\nabla^2 H_0 = \delta\nabla^2\Phi_0. \tag{20}$$

To formulate the problem in terms of the variable ξ, one needs to make the transformation in Eqs. 19 and 20 via one of the following substitutions: $\nabla f \equiv (f', 0)$, and $\nabla(g, 0) \equiv g'$ for the case of plane heat source, or $\nabla(g, 0) \equiv (rg)'/r$ for the axisymmetrical hot spot. Here f and g are arbitrary scalar functions, the prime denotes the derivative with respect to ξ, and (p, s) indicates a vector in the orthogonal coordinate system, whose first component is aligned with the ξ-axis.

Equations 19 and 20 determines the basic state solution of the evolutionary system (13)–(15) depending on the

parameters of fluid (Prandtl or Schmidt number) and the parameters of local heating or introduced surfactant (16) and (17). To analyze the main properties and possible simplifications of Eqs. 19 and 20, consider the case of plane heat flux inhomogeneity (hot bar), for which the equations of base state read:

$$a_1\Phi''''(x) - H''(x) - a_2((\Phi'(x))^3)' + a_3(\Phi'(x)\Phi''(x))' + \\ + a_4((\Phi'(x))^2)'' + a_5(H(x)\Phi'(x))' - \\ - (q(x)\Phi'(x))' + a_6 q''(x) + \xi q(x)H(x) = 0 \\ H''''(x) - \delta H''(x) - c\Phi''(x) = 0 \tag{21}$$

For certain limit cases it is possible to simplify the equations. Namely, for the approximation of non-derformable surface ($H = 0$) we get one equation of the fourth order:

$$a_1\Phi''''(x) - a_2((\Phi'(x))^3)' + a_3(\Phi'(x)\Phi''(x))' + \\ + a_4((\Phi'(x))^2)'' - (q(x)\Phi'(x))' + a_6 q''(x) = 0 \tag{22}$$

On setting $a_3 = a_4 = a_6 = 0$ in Eq. 21, we get the same governing equations as those obtained in the long-wave approximation for thermal convection in the locally heated layer (Lyubimov and Tcherepanov 1991). Substituting $N(x) = \Phi'(x)$ and using the decay of all variables at $x \to \pm\infty$ one obtains:

$$a_1 N''(x) - a_2 N^3(x) + (a_3 + 2a_4)N(x)N'(x) \\ - q(x)N(x) + a_6 q'(x) = 0. \tag{23}$$

The Eq. 23 (with $a_6 = 0$) is actually the nonlinear spatial Schrödinger equation with the potential $q(x)/a_1$.

To obtain the solution of the general system (13)–(15) and its further simplifications, setting the appropriate boundary conditions is required for $\Phi_0(\xi)$, $H_0(\xi)$, and their derivatives at the center of "hot spot" and at infinite value of the argument. In terms of the amplitude functions, the boundary conditions are written down in the form:

a) for the planar problem:

$$\Phi(x, t) \to 0, \partial_x\Phi(x, t) \to 0, H(x, t) \to 0, \\ \partial_x H(x, t) \to 0, \ x \to \pm\infty \tag{24}$$

b) for the axisymmetrical problem

$$\Phi(r, t) \to 0, \partial_r\Phi(r, t) \to 0, \partial_{rr}^2\Phi(r, t) \to 0, \\ H(r, t) \to 0, \partial_r H(r, t) \to 0, \partial_{rr}^2 H(r, t) \to 0, \ r \to +\infty \\ \partial_r\Phi(r, t) = 0, \partial_r H(r, t) = 0, r = 0. \tag{25}$$

The main technique for solving stationary nonlinear amplitude equations for the plane and axisymmetric variants of the problem has been the Galerkin method. For each of the variants, a set of appropriate basic functions has been used. The main feature of the method is the choice of basic functions that are defined on the whole domain of definition and satisfy the boundary conditions.

In the planar case, the whole abscissa is the domain of the definition, so the coordinate transformation was performed in the first stage of the solution, which reduced the infinite domain of definition to the finite one, specifically:

$$\gamma = \tanh(\beta \cdot x); \quad x \in (-\infty, \infty) \rightarrow \gamma \in [-1, 1].$$

In the transformed coordinates, the basic functions and decomposition of the unknown variables have the form:

$$\{\gamma^k\}_{k=0,1,2,..}; \ \Phi_0 = \sum_k \alpha_k \cdot \gamma^k; \ H_0 = \sum_k \beta_k \cdot \gamma^k$$

On the new boundaries, only zero boundary condition for all functions is applied. The remaining boundary conditions are completely satisfied by the basis functions themselves. To search for axisymmetric stationary solutions, coordinate transformation is not performed. The basic functions in this case have the form:

$$\left\{ 1 \big/ (r+1)^i \right\}; \ i = 1, 2, \ldots$$

They are defined on the semi-line and satisfy the boundary conditions at infinity. The basis functions do not satisfy the boundary conditions at the origin.

Further, following the general methodology of the Galerkin method and using the minimum condition of the mismatch, the differential equations were reduced to nonlinear algebraic equations, the unknowns being the coefficients of the basis functions in the representation of the unknown functions. Linear algebraic equations obtained from boundary conditions are added to these equations. At the last stage the system of algebraic equations was solved by the methods of direct numerical integration realized in the package Mathematica. For finding the complete set of the solutions of the system of nonlinear algebraic equations in the stationary case the Bukhberger's algorithm (Cox et al. 2007), based on the finding of the Gröbner basis, and different iteration techniques of the solution are used. The solution of the initial value problem in the nonstationary case is obtained by the Runge-Kutta methods of different orders.

Dependence of the numerical solution on the number of basis functions was investigated. Already with 5 basis functions, convergence is observed.

Linear Analysis of Stability of the Basic State

In accordance with the general approach of linear theory of hydrodynamic stability, we follow the propagation of the small normal perturbations of steady state given by Eq. 18:

$$\begin{aligned}
\Phi(x, y) &= \Phi_0(x, y) + \Phi'(x, y)e^{\lambda t}; \\
\Psi(x, y) &= \Psi_0(x, y) + \Psi'(x, y)e^{\lambda t}; \\
H(x, y) &= H_0(x, y) + H'(x, y)e^{\lambda t}.
\end{aligned}$$

After substituting this form of solution in Eqs. 13–15 and the linearization we get the following spectral problem (primes at the perturbation terms are omitted):

$$\begin{aligned}
&\lambda\Phi + a_1\nabla^4\Phi - \nabla^2 H - 3a_2\nabla\left(|\nabla\Phi_0|^2\nabla\Phi\right) \\
&+ a_5\nabla(H_0\nabla\Phi + H\nabla\Phi_0) + a_3\nabla\left(\nabla^2\Phi_0\nabla\Phi + \nabla^2\Phi\nabla\Phi_0\right) \\
&+ \nabla\Phi_0 rot(\vec{e}_z\Psi) + 2a_4\nabla^2|\nabla\Phi_0\nabla\Phi| - \nabla(q\nabla\Phi) = 0;
\end{aligned} \tag{26}$$

$$\begin{aligned}
&b_1\left(\nabla(\Delta\Phi_0)\times\nabla\Phi + \nabla(\Delta\Phi)\times\nabla\Phi_0\right) - b_2(\nabla H_0 \\
&\times\nabla\Phi - \nabla H\times\nabla\Phi_0) - \vec{e}_z\Delta\Psi = 0;
\end{aligned} \tag{27}$$

$$\nabla^4 H - c\nabla^2 H = \delta\nabla^2\Phi. \tag{28}$$

The problem (26)–(28) is non-selfadjoint, and in the general case admits the excitation of instability with respect to disturbances of both monotonic or oscillatory types.

However, in the case of stepwise heat flux inhomogeneity the basic state can be approximately considered as equilibrium. This becomes possible due to the condition $\nabla^2 q = 0$, valid at almost all x, except for the edges of the step, and permitting to set $\Phi_0(\xi) = H_0(\xi) = 0$ in Eqs. 19 and 20. Linear analysis is simplified in this case, and discloses only the monotonic instability (Wertgeim and Myznikova 2002).

We seek the small perturbation functions in the following form:

a) in the planar case:
$\Phi(x, y, t) = \phi(x, t)\cdot e^{i\cdot k_y\cdot y}$; $H(x, y, t) = h(x, t)\cdot e^{i\cdot k_y\cdot y}$; $\Psi(x, y, t) = \psi(x, t)\cdot e^{i\cdot k_y\cdot y}$ Here k_y is the wave number along the coordinate orthogonal to the one on which the fundamental solution depends.

b) in the axisymmetric case:.
$$\begin{aligned}
\Phi(r, \varphi, t) &= \phi(r, t)\cdot e^{i\cdot m\cdot\varphi}; \ H(r, \varphi, t) \\
&= h(r, t)\cdot e^{i\cdot m\cdot\varphi}; \ \Psi(r, \varphi, t) \\
&= \psi(r, t)\cdot e^{i\cdot m\cdot\varphi}.
\end{aligned}$$

Here m is the wavenumber along the azimuthal coordinate.

As a result, we obtain partial differential equations for functions that contain two independent variables.

These equations have been solved by finite difference methods. Approximation of partial derivatives with respect to the spatial coordinate is of the second order. As a result, we derive the ODE system with the number of equations proportional to the number of nodes in the grid. The ODE solution was computed by the explicit adaptive method of the first-order with respect to the time, which is adequate for the problem due to the absence of sharp changes in the temporal evolution of the perturbation. During the integration process, the timestep has been automatically

varied. The initial perturbation had the form of a localized function with one extremum. Further evolution of this disturbance has been considered, whereby the stability or instability of the basic state has been revealed and the decrement or increment has been determined.

Methods of Solution for 2D Problem

The problem in the complete 2D nonlinear formulation (13)–(15) is treated numerically using the semi-implicit pseudo-spectral approach developed for nonlinear thermo-capillary convection in the uniformly heated layer (Nepom-nyashchy et al. 2002).

The nonlinear convective terms in Eqs. 13–15 are calculated via transformation from the Fourier coefficient space to the physical space, and vice versa. Temporal evolution of the Fourier coefficients has been calculated by finite-difference technique using the Crank-Nicolson discretization scheme for the linear terms and the Adams-Bashforth method for the nonlinear terms.

Initial conditions of two specific types were tested. The first variant corresponded to the supercritical pattern of spatially periodic convective rolls known from the case of uniform heating. For the second version the 1D steady-state solution with an inhomogeneous heating, obtained earlier for other parameter values, was chosen as the starting state.

The boundaries of stability of the basic state with respect to the disturbances of different types have been located numerically.

Basic State Simulations: Influence of Heat Flux $Q(\xi)$

The main aim of the studies has been to investigate the influence of applied heat inhomogeneity upon the basic stationary solutions of Eqs. 19 and 20. Let us start with solutions of small amplitude deduced from Eqs. 19 and 20 by neglecting nonlinear terms. Calculations for different forms and parameters of $q(\xi)$ have been performed. The dependence of the amplitude of the temperature perturbation $\Phi_0(0)$ on the parameter of the heat flow inhomogeneity α, characterizing intensity of local heating, is demonstrated in Fig. 1.

One can see that the shape of solution and its characteristic amplitude at the center of the hot spot depend substantially on the parameter α. At small values of α, the amplitude of temperature is bell-shaped and takes only negative values. As α increases, the amplitude decreases until some critical value of α is reached. At this point, the dependence develops a discontinuity of the second kind. A further increase in the parameter leads to change of the
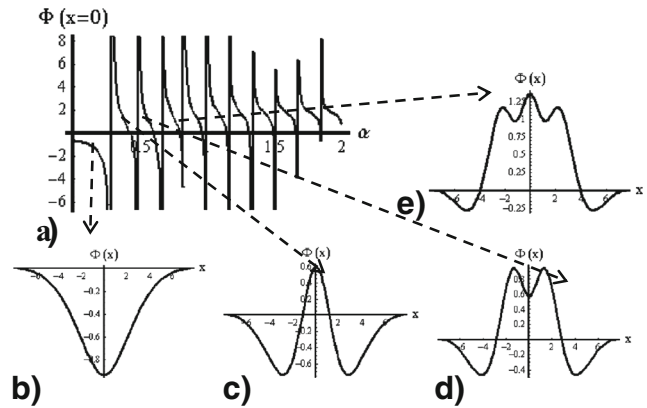

Fig. 1 The value of the temperature amplitude at the center of the spot (**a**) and its shape (**b-e**) as function of the parameter α (0.1 (**b**), 0.4 (**c**), 0.58 (**d**), 0.75 (**e**)), β =0.3, the heat flux type I, planar case)

sign of temperature amplitude at the center of the thermal spot, and this is repeated many times as the parameter grows. At the same time, the number of local extrema of the temperature distribution function increases. Noteworthy that the length of the regions between the critical values remains almost constant:

$$\alpha_2 - \alpha_1 \approx \alpha_3 - \alpha_2 \approx ... \approx const. \tag{29}$$

This behavior turns out to be typical not only for Eqs. 19–20, but also for all simplifications (21)–(23), in particular for the case of the non-deformable boundary ($c = \delta = 0$), and for its further reduction to a boundary-value problem for the spatial Schrödinger equation, obtained after linearization of Eq. 23, with the potential $q(x)/a_1$. Assuming an infinite interval of definition and the decay of the unknown variables on infinitely remote boundaries, one gets the exact analytic solution of the linearized problem (23) (Landau and Lifshits 1977):

$$N(x) = (1 - \tanh^2(\beta x))^{\frac{1}{2}} F\left(1 - s, 2 + s, 2, \frac{1 - \tanh(\beta x)}{2}\right);$$
$$s = \frac{1}{2}\left(-1 + \sqrt{1 + 4\frac{\alpha^2 + \beta^2}{\beta^2}}\right) \tag{30}$$

In the formula (30) F is the hypergeometric function, s is the parameter of its arguments. Solutions are localized only for the discrete set of parameters α and β, obeying the relation: $\alpha_n = \beta_n \sqrt{n^2 + 3n + 1}$. These solutions differ in the number of extrema, the first three of them are shown on Fig. 2.

Within the above problem formulation, there are no discontinuities of the second kind in the dependence of localized solution (30) on α, but the required zero boundary conditions at infinity are satisfied only for certain discrete values of the parameters α_n and β_n, $n = 0, 1, 2...$, whereas
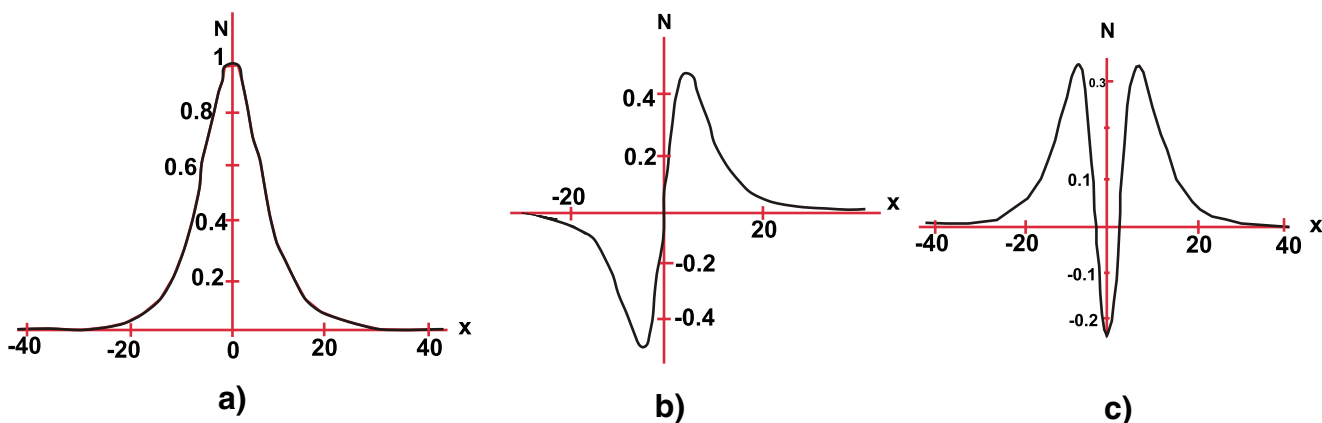
Fig. 2 Solutions (30) for n=0 (**a**), n=1 (**b**), n=2 (**c**) (β =0.2, heat flux type I, planar case)

for other values of these parameters the solution grows unlimitedly at one end of the interval. However, if in the numerical simulation of the boundary value problem it is compulsory to require the fulfillment of zero boundary conditions at infinity for all α and β, the discontinuities of the second kind appear at the corresponding critical values $\tilde{\alpha}_n \approx \alpha_n$. Note that the exact solution (30) corresponds to case of heat flux of type I, and one can see from expression for critical values α_n that approximate relations (29) are

valid. For the other investigated form of the heat flow, type II (13), all described properties of the solution are preserved, except that the lengths of the regions between the critical values do not remain constant and grow with increase of α : $\alpha_2 - \alpha_1 < \alpha_3 - \alpha_2 < ...$ (Fig. 3).

In the numerical study of the initial nonlinear boundary value problems (18)–(22) the unknown variables demonstrate similar behavior. The critical values of parameters α (or β), corresponding to sharp transitions between different
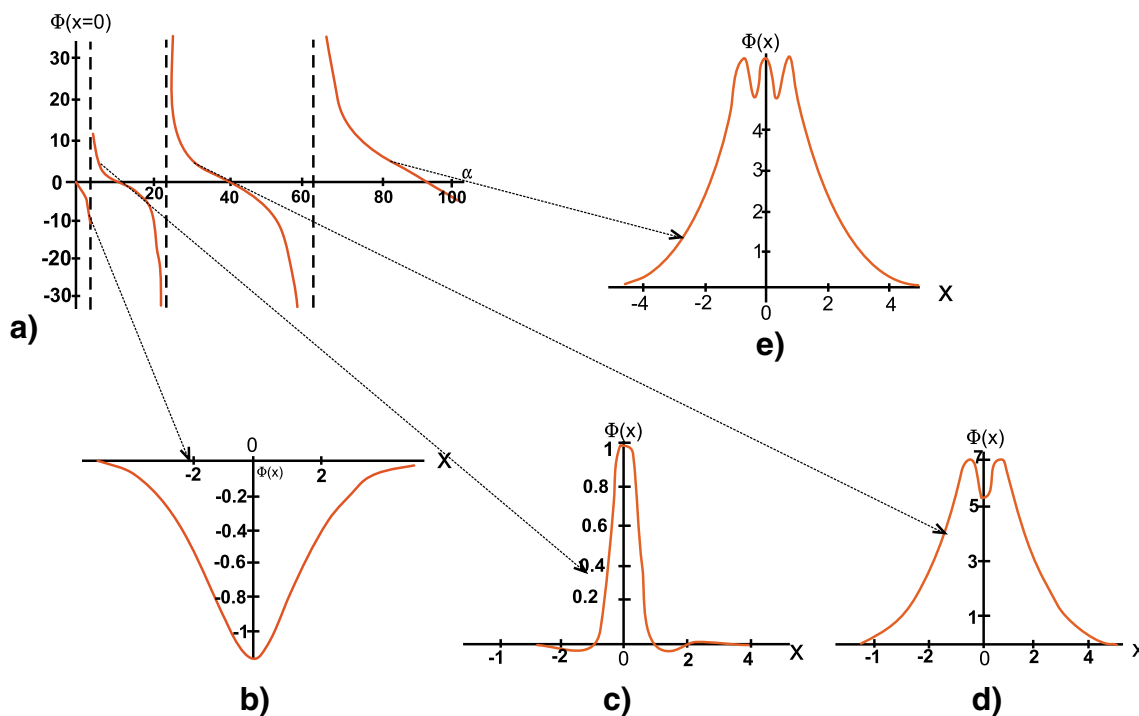

Fig. 3 The value at the center of the spot (**a**) and the shapes (**b**)–(**e**) of the temperature amplitude as function of the parameter α, (β =0.2, heat flux type II, planar case)

shapes of solutions persist, with slightly changing numerical values. Instead of discontinuity of the second kind, a narrow transition region with finite values of variables on its boundaries appears.

Variation of other parameters of the problem (19) and (20) leads to the same kind of dependencies. This is valid, in particular, for dependence on the inverse capillary number: parameter c. The regions of sharp changes in shape and amplitude of the variables, and the number of local extrema of functions increases when passing through the critical value of the parameter. The characteristic features of the dependences of the temperature distribution and the shape of the surface on the parameters of thermal inhomogeneity and the properties of the liquid are confirmed by experimental observations of various stages of the process of heating the liquid layer by localized radiation, produced by a laser beam (Karlov et al. 2005) or incoherent light source (Mizev 2004), depending on the change in the thickness of the layer, the size and power of the thermal inhomogeneity source.

For the nonlinear equations, in contrast to the linear ones, the presence of the multiple solutions is typical. The dependences of the amplitude of steady-state solutions of nonlinear problem on the parameter α at different β for heat flux type I, planar case, are represented in Fig. 4.

For the small β this dependences at large scales are straight lines filling the cone-shaped region (Fig. 4a). With β values larger than $\beta \sim 10$ the multiplicity of solutions is typical only for the region of small $\alpha \in [0, \alpha_*]$, in this case $\alpha_* \approx 60$. Outside this region at $\alpha > \alpha_*$ there is a unique
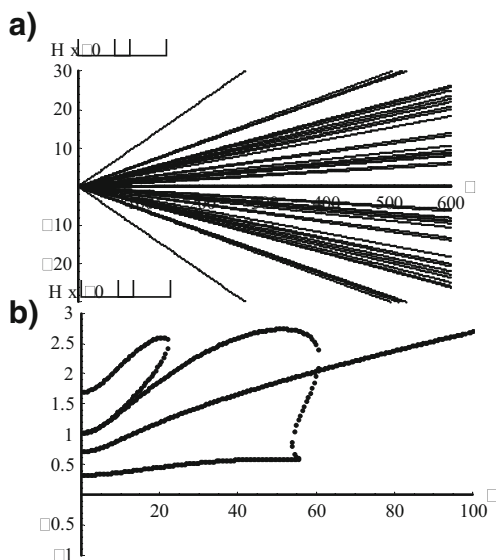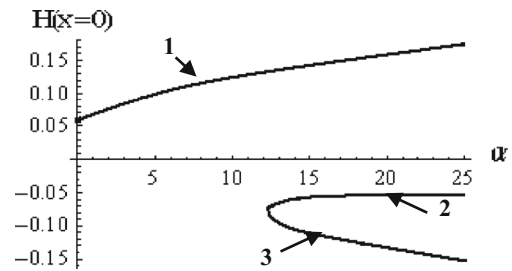

Fig. 5 Dependence of the value of the amplitude of the deformation of the surface in the center of the thermal spot on the heat flux parameter α. $\beta = 7$, $c = 0.1$, $\delta = 0.1$, $Pr = 13$, $\zeta = 0$, $R = 1$

solution (Fig. 4b). All the features described above persist also in the case of axisymmetrical inhomogeneity of heat flux.

Stability of the Basic States: Numerical Results

For the nonstationary thermal source, corresponding to the experimental situation of the gradual increase of the power of laser radiation up to the specific value within the specified time interval (Karlov et al. 2005), the parametric domains are investigated, where either the processes of the establishment of steady state or the nonstationary passages between them take place, and their dependences on the warmup time and spatial inhomogeneity of thermal source are studied.

Due to the above mentioned multiplicity of solutions of equations for basic states, it is worth to consider in the stability analysis of basic states (19) and (20), using (26)–(28), not the single stationary solution, but the whole branch depending on some parameter. Figure 5 shows the dependence of the amplitude of deformation of stationary basic state on the heat flux parameter α for the planar case. It should be noted that for all values of this parameter there

Fig. 4 Dependences of steady solutions of planar nonlinear problem on the parameter α (**a**: $\beta = 1$; **b**: $\beta = 10$)
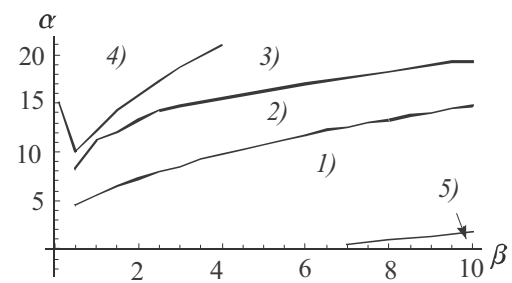

Fig. 6 Stability map of the main planar steady states. The regions on the map correspond to the existence: two paired branches of unstable states (2, 3, 4); Stability of the unit branch: **a** for $k_y = 0$, the regions 1, 2, 5; **b** for $k_y = 1$, the regions 1, 2, 3
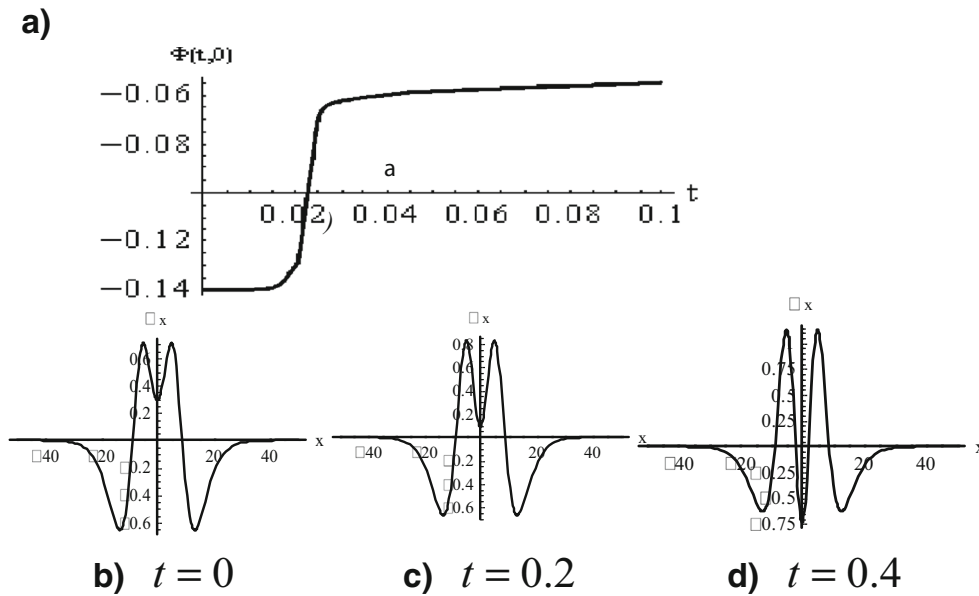
Fig. 7 Non-stationary solution of the nonlinear problem for initial state with parameters $\alpha = 0.3$, $\beta = 0.1$, c $= \delta = 1$, $\varsigma = -0.015$, Pr=13 **a** time dependence $\Phi(0, t)$; **b-d** - horizontal profiles $\Phi(\xi, t)$ at different moments of time

is a solitary branch marked 1 in the Figure. Starting from a certain value of α, a further pair of branches appears, whereas the basic states corresponding to these branches coincide in form and differ in sign.

Results of stability analysis of plane basic states with respect to small perturbations described above (with $k_y \in [0, 1]$) are presented in Fig. 6, where the area of existence of the pair of branches is indicated by the numbers 2 and 3. The steady states on these branches are unstable, with the steady states on the lower branch being monotonically

unstable, and those on the upper one being oscillatory unstable in the entire region of existence. On the solitary branch there are both stable and unstable steady states, depending on the transversal wavenumber k_y. The complete study of dependence of stability on this parameter is not yet accomplished, but from Fig. 6 it can be inferred for two values of k_y. The regions of stability are 1, 2, 5 for $k_y = 0$, and 1, 2, 3 for $k_y = 1$. As can be seen, in the case $k_y = 1$ for small α and finite β, steady states on the solitary branch become unstable.

Fig. 8 Dependence of stationary solutions of nonlinear axisymmetric problem on the parameter α at $\beta = 0.1$ (solid lines – stable solutions, dashed lines – unstable ones)
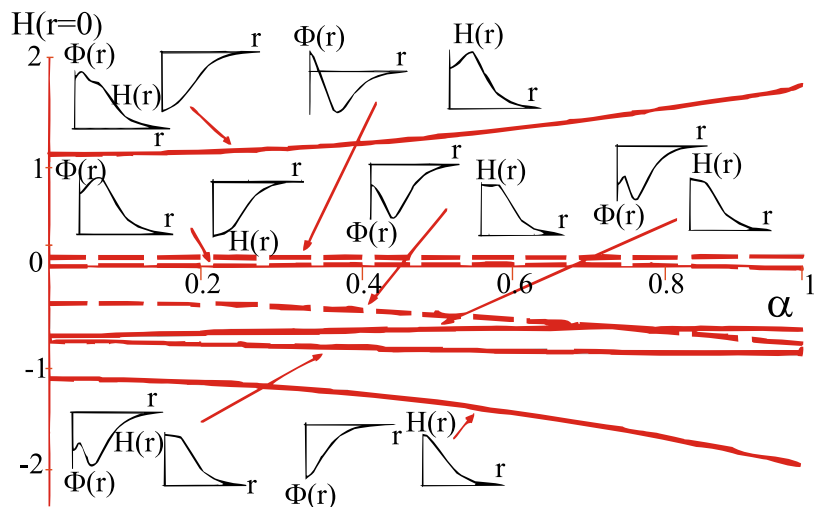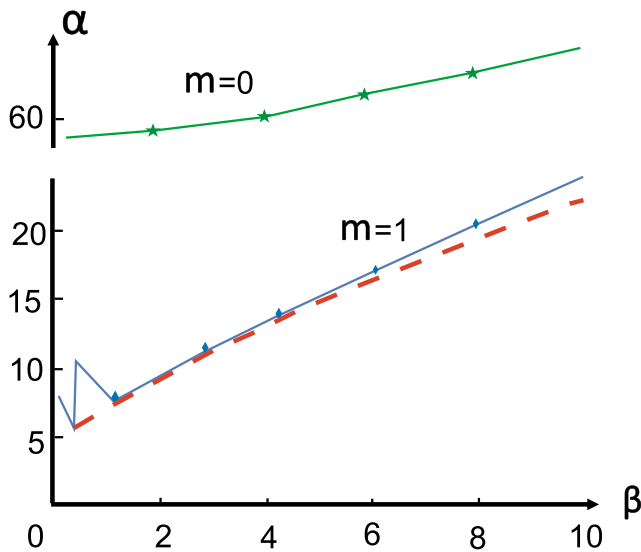
Fig. 9 Stability map for steady states in axisymmetric problem. Stability boundaries for axisymmetric (m=0) and dipole (m=1) modes. Dashed line: axisymmetric basic solution

cellular structures in the entire space, occupied with liquid. The results of 2D calculations confirm the presence of the global and local modes of instability, previously forecasted by linear theory, and they also demonstrate the possibility of oscillatory regimes (Fig. 10).
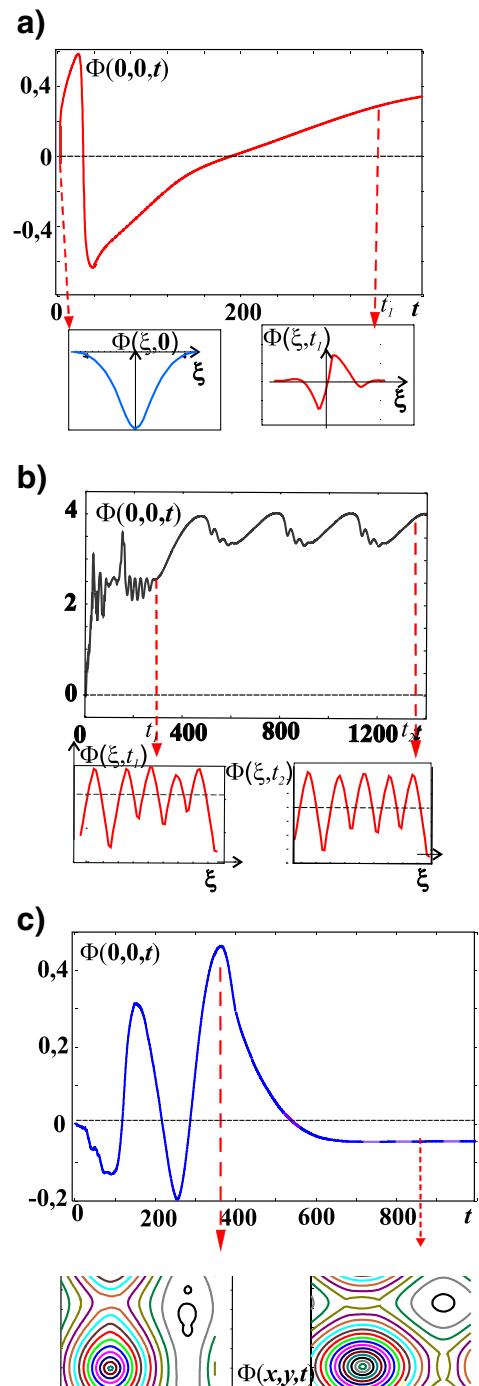

Fig. 10 Development of the disturbances of temperature for the different modes of the instability of the one-dimensional stationary solutions: 1D local monotonic mode (**a**), 1D global oscillating mode (**b**) and 2D mode (**c**) (planar thermal heterogeneity)

As an alternative way, the numerical analysis of the stability of steady state solutions is performed. Solutions of the nonstationary problem (13)–(15) in 1D version are found using the Galerkin method, starting from one of previously obtained steady solutions and adding some small perturbation. Further development of the perturbation is demonstrated in Fig. 7.

For the axysymmetric problem, like in the planar case (Figs. 5 and 7), multiple solutions at the fixed parameters are found, differing between themselves by the number of local extrema (Fig. 8). The most dangerous instability mode for these solutions is typically the dipole one for a wide range of parameters (Fig. 9).

For the analysis of stability of the obtained steady states to 2D disturbances, the study of their nonlinear development on the basis of solution of the complete 2D problem (13)–(15) by the pseudo-spectral method has also been executed (Karlov et al. 2005; Wertgeim et al. 2013). Numerical results showed that the obtained one-dimensional stationary solutions are stable and are encountered in a certain range of the parameters. Qualitatively the stability region can be determined from the results of linear theory in the approximation of zero steady-state solution (Wertgeim and Myznikova 2002), for the more precise determination it is necessary to examine the complete problem of stability of the non-zero solutions. Beyond the limits of stability region, the 2D calculations demonstrate the development of both the localized disturbances of another symmetry (in the planar case - with the odd profile of dependences, in the axisymmetrical one – the disturbance with dipole pattern), and the disturbances, which lead to the global

Conclusions

Results of numerical studies show that inhomogeneous surface tension, created by either localized heat flux or localized deposition of surfactant, has a significant effect on the Marangoni convection in a thin liquid layer with a deformable surface, leading to a large variety of spatial patterns in the fluid flow, temperature distribution and surface deformation. For sufficiently small values of the layer thickness, it is possible to use long-wave approximation, which simplifies the problem considerably.

Analysis of the basic states and their stability showed that their properties depend significantly on the parameters of the spatial inhomogeneity of surface tension and physical parameters of the system, with sharp transitions between different forms of solution at certain parameter values.

The results of nonlinear numerical experiments confirm the existence and types of instability modes predicted by the linear stability analysis. They allow us to describe the evolution of disturbances far from the threshold of the instability excitation, to study transitions between different structures of thermo-capillary flow, and peculiarities of heat transfer.

The results correspond qualitatively to the regimes and spatial structures of thermocapillary convection observed in experiments based on localized heating of the liquid layer. For a better quantitative correspondence and description of the observed oscillatory and wave modes it is necessary to take into account, in the modified mathematical model, the finiteness of the magnitude of the thermal inhomogeneity, the three-dimensional nature of the flow, the temperature distribution and deformation of the surface, and the effect of thermogravitational convection.

It is shown that the noted characteristic features of the behavior of solutions are mostly preserved in simplified formulations obtained from the complete nonlinear problem, in particular, by its linearization or in the approximation of the absence of deformation of the boundary.

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