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NUMERICAL SIMULATION OF MICROCONVECTION IN DOMAINS WITH FREE BOUNDARIES

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1. Introduction. The Oberbeck–Boussinesq system of equations is usually used to describe free gravitational or thermocapillary convection. Analyzing the assumptions made in the derivation of this system from the exact equations of continuum mechanics, V. V. Pukhnachev [1] have shown that the classical model cannot be applied to convection in small domains and in weak gravity or fast-varying temperature fields. In [2], Perera and Sekerka have noted the interest in new models of convection and a need for replacement of the conventional model for microconvection in fluids. In [3, 4], the author investigated numerically fluid flows in domains with fixed boundaries under the action of microaccelerations attainable aboard a space vehicle with the use of the classical model of convection and the new model of Pukhnachev. The qualitative and quantitative differences in the flow characteristics were verified. In the new model of microconvection, the equations of conservation of mass and momentum are satisfied exactly, and the equation of energy is satisfied asymptotically. When the specific volume $1/\rho$ depends linearly on the temperature, the initial system of equations is transformed into a system in which the modified velocity vector becomes solenoidal. This makes it possible to introduce a stream function for plane and axially symmetric problems and to calculate convective flows in stream function–vorticity variables.

In the present paper, the steady two-dimensional thermocapillary gravitational convection in annular domains with free boundaries is investigated numerically. The free boundaries can then be considered rigid and approximately defined as the surfaces of capillary equilibrium under conditions of zero gravity and with a rather small parameter responsible for deformation of the free surfaces by thermocapillary forces (capillary number). The free boundaries are corrected by their dynamic conditions. Calculations were carried out by the method tested in the above-mentioned studies of free convection and microconvection in fixed domains.

2. Formulation of the Problem. The steady gravitational capillary convection is investigated in the annular domain $0 < R_1 \leqslant r \leqslant R_2 < +\infty$, $0 \leqslant \varphi \leqslant 2\pi$ for two cases:

(1) for $I = 0$, we have heat transfer through the fixed inner boundary ($r = R_1$) and heat insulation of the free outer boundary ($r = R_2$);

(2) for $I = 1$, we have heat transfer through the fixed outer boundary ($r = R_2$) and heat insulation of the free inner boundary ($r = R_1$).

The equations of convection are considered here in nondimensional form. In this case, the following characteristic size, velocity, temperature, and pressure are introduced: $l = R_0 - R_1$, $\gamma T_0/\mu$, T_0, and $\gamma T_0/l$, where γ is the temperature coefficient of surface tension, T_0 is the characteristic temperature difference, and μ is the dynamic viscosity (see, for example, [5]).

• *Classical Oberbeck–Boussinesq Model* (OBM). The stream function ψ, the vorticity ω, and the temperature T in the polar coordinates (r, θ) satisfy the following system:

$$\Delta\omega - \mathrm{Re}\Big(v\frac{\partial\omega}{\partial r} + \frac{u}{r}\frac{\partial\omega}{\partial\varphi}\Big) - \frac{\mathrm{Gr}}{\mathrm{Ma}}\Big(\frac{\partial T}{\partial r}\cos\varphi - \frac{1}{r}\frac{\partial T}{\partial\varphi}\sin\varphi\Big) = 0; \tag{2.1}$$

$$\Delta\psi + \omega = 0; \tag{2.2}$$

$$\Delta T - \mathrm{Ma}\Big(v\frac{\partial T}{\partial r} + \frac{u}{r}\frac{\partial T}{\partial\varphi}\Big) = 0. \tag{2.3}$$

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Here $\mathrm{Re} = l\gamma T_0/\mu\nu$, $\mathrm{Ma} = \mathrm{Re}\,\mathrm{Pr}$, $\mathrm{Pr} = \nu/\chi$, and $\mathrm{Gr} = g\beta T_0 l^3/\nu\chi$ are the Reynolds, Marangoni, Prandtl, and Grashof numbers, respectively; ν is the kinematic viscosity, χ is the thermal conductivity, g is the acceleration of gravity, β is the volume coefficient of thermal expansion, $\beta T_0 = \mathrm{Gr}/\mathrm{Pu}$ ($\mathrm{Pu} = gl^3/\nu\chi$ is the Pukhnachev number), $u = r^{-1}\partial\psi/\partial\varphi$ is the radial velocity component; and $v = -\partial\psi/\partial r$ is the tangential velocity component.

The boundary conditions are as follows:
for $I = 0$

$$r = R_1: \quad \psi = 0, \quad \frac{\partial\psi}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = H\cos\varphi \quad (H = \mathrm{const}),$$

$$r = R_2: \quad \psi = 0, \quad R_2\omega + 2\frac{\partial\psi}{\partial r} = -\frac{\partial T}{\partial\varphi}, \quad \frac{\partial T}{\partial r} = 0,$$

and for $I = 1$

$$r = R_1: \quad \psi = 0, \quad R_1\omega + 2\frac{\partial\psi}{\partial r} = -\frac{\partial T}{\partial\varphi}, \quad \frac{\partial T}{\partial r} = 0,$$

$$r = R_2: \quad \psi = 0, \quad \frac{\partial\psi}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = H\cos\varphi.$$

• *New Model* (NM). For the functions ψ, ω, and T, the nondimensional equations in polar coordinates are as follows:

$$(1+\beta T_0 T)\Delta\omega - \mathrm{Re}\Big(v\frac{\partial\omega}{\partial r} + \frac{u}{r}\frac{\partial\omega}{\partial\varphi}\Big) + \beta T_0\Big\{\frac{1}{r}\frac{\partial T}{\partial\varphi}\frac{\partial q}{\partial r} - \frac{1}{r}\frac{\partial T}{\partial r}\frac{\partial q}{\partial\varphi} + \Big[\frac{\partial T}{\partial r}\Big(\Delta u - \frac{u}{r^2}\Big) - \frac{1}{r}\frac{\partial T}{\partial\varphi}\Big(\Delta v - \frac{v}{r^2}\Big)\Big]\Big\}$$
$$- \frac{\mathrm{Gr}}{\mathrm{Ma}}\Big(\frac{\partial T}{\partial r}\cos\varphi - \frac{1}{r}\frac{\partial T}{\partial\varphi}\sin\varphi\Big) - \frac{\beta T_0}{\mathrm{Pr}}\Big\{\omega\Delta T + \frac{\partial T}{\partial r}\frac{\partial\omega}{\partial r} + \frac{1}{r^2}\frac{\partial T}{\partial\varphi}\frac{\partial\omega}{\partial\varphi}\Big\}$$
$$- \frac{\beta^2 T_0^2}{\mathrm{MaPr}}\Big\{\frac{1}{r}\Big(-\frac{\partial T}{\partial r}\frac{\partial\Delta T}{\partial\varphi} + \frac{\partial T}{\partial\varphi}\frac{\partial\Delta T}{\partial r}\Big)\Big\} = 0; \tag{2.4}$$

$$\Delta\psi + \omega = 0; \tag{2.5}$$

$$(1+\beta T_0 T)\Delta T - \mathrm{Ma}\Big(v\frac{\partial T}{\partial r} + \frac{u}{r}\frac{\partial T}{\partial\varphi}\Big) - \beta T_0|\nabla T|^2 = 0. \tag{2.6}$$

Here ψ is a modified stream function [1]. For the new model, the boundary conditions are as follows:
for $I = 0$

$$r = R_1: \quad \psi = -R_1\frac{\beta T_0}{\mathrm{Ma}}H\sin\varphi, \quad \frac{\partial\psi}{\partial r} = \frac{1}{R_1}\frac{\beta T_0}{\mathrm{Ma}}\frac{\partial T}{\partial\varphi}, \quad \frac{\partial T}{\partial r} = H\cos\varphi,$$

$$r = R_2: \quad \psi = 0, \quad \omega + \frac{2}{R_2}\frac{\partial\psi}{\partial r} = \frac{\partial T}{\partial\varphi}\Big(2\frac{\beta T_0}{\mathrm{Ma}}\frac{1}{R_2^2} - \frac{1}{R_2}\Big), \quad \frac{\partial T}{\partial r} = 0,$$

and for $I = 1$

$$r = R_1: \quad \psi = 0, \quad \omega + \frac{2}{R_1}\frac{\partial\psi}{\partial r} = \frac{\partial T}{\partial\varphi}\Big(2\frac{\beta T_0}{\mathrm{Ma}}\frac{1}{R_1^2} - \frac{1}{R_1}\Big), \quad \frac{\partial T}{\partial r} = 0,$$

$$r = R_2: \quad \psi = -R_2\frac{\beta T_0}{\mathrm{Ma}}H\sin\varphi, \quad \frac{\partial\psi}{\partial r} = \frac{1}{R_2}\frac{\beta T_0}{\mathrm{Ma}}\frac{\partial T}{\partial\varphi}, \quad \frac{\partial T}{\partial r} = H\cos\varphi.$$

Corrections to the free surface can be calculated in the following manner: let $h(\varphi)$ be the deviation of the free surface from $r = R_1$ (or $r = R_2$). For $\mathrm{Ca} = \gamma T_0/\sigma_0 \to 0$ and $\mathrm{Gr}/\mathrm{Ma}(\beta T_0) \to 0$, the balance of the normal stresses at the inner (outer) boundary then yields

$$\delta P - 2\frac{\partial v}{\partial r} = \pm\Big\{-(T - T_*)\frac{1}{R} - \frac{1}{\mathrm{Ca}}\frac{(h + h'')}{R^2}\Big\} - \frac{\mathrm{Gr}}{\mathrm{Ma}(\beta T_0)}R\sin\varphi, \quad R = R_1(R_2),$$

TABLE 1

Substance	Pr	Ma	Re	Gr	Pu	βT_0	Gr/Ma	βT_0/Pr	$\beta^2 T_0^2$/MaPr
Glycerin	10^4	$3 \cdot 10^2$	$3 \cdot 10^{-2}$	$1.5 \cdot 10^{-3}$	10^{-1}	$1.5 \cdot 10^{-2}$	$5 \cdot 10^{-6}$	$1.5 \cdot 10^{-6}$	10^{-10}
	10^4	1	10^{-4}	$0.5 \cdot 10^{-5}$	10^{-1}	$0.5 \cdot 10^{-4}$	$5 \cdot 10^{-6}$	$0.5 \cdot 10^{-8}$	10^{-12}
Glass	10^4	10	10^{-3}	$0.5 \cdot 10^{-6}$	10^{-2}	$4.5 \cdot 10^{-5}$	$5 \cdot 10^{-8}$	$4.5 \cdot 10^{-9}$	10^{-14}
Silicon	$4 \cdot 10^{-3}$	1	$2.5 \cdot 10^2$	$0.3 \cdot 10^{-7}$	1	$0.3 \cdot 10^{-7}$	$0.3 \cdot 10^{-7}$	$0.8 \cdot 10^{-5}$	10^{-13}

TABLE 2

Substance	Pr	Ma	Re	Gr	Pu	βT_0	Gr/Ma	βT_0/Pr	$\beta^2 T_0^2$/MaPr
Glycerin	10^4	1	10^{-4}	$1.5 \cdot 10^{-3}$	10^{-1}	$1.5 \cdot 10^{-2}$	$1.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-6}$	$1.8 \cdot 10^{-8}$
Silicon	$4 \cdot 10^{-3}$	1	$2.5 \cdot 10^2$	$2 \cdot 10^{-4}$	1	$2 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$5 \cdot 10^{-2}$	10^{-5}

where $(\ )' = d/d\varphi$; δP is the pressure deviation from the equilibrium level $\delta P_0 = 1/(\mathrm{Ca}R)$ for $\gamma = 0$ and $g = 0$.

3. Numerical Investigation. We introduce a difference grid $r_n = R_1 + (n-1)h$ $(n = 1, \ldots, N+1)$, $h = (R_2 - R_1)/N$, $\varphi_m = (m-1)\alpha$ $(m = 1, \ldots, M+1)$, $\alpha = 2\pi/M$, and $f_{n,m} = f(r_n, \varphi_m) = f_{n,m+M}$.

The problems formulated for Eqs. (2.1)–(2.3) and (2.4)–(2.6) are investigated numerically by the method of reaching a steady state with the use of a longitudinal-transverse finite-difference scheme. For Eqs. (2.1) and (2.3) or (2.4) and (2.6), this scheme can be written in the following general form:

$$(U^{k+1/2} - U^k)/0.5\tau = \lambda_k[\Lambda_1 U^k + \Lambda_2 U^{k+1/2} + F^{k+1/2}],$$

$$(U^{k+1} - U^{k+1/2})/0.5\tau = \lambda_k[\Lambda_1 U^{k+1} + \Lambda_2 U^{k+1/2} + F^{k+1/2}].$$

Here $U = \binom{\omega}{T}$, $U^k = U(t^k)$, Λ_1 and Λ_2 are difference operators which approximate, respectively, the following differential operators

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}, \qquad \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2},$$

and λ_k is an iteration parameter.

To solve Eqs. (2.2) or (2.5), at each iteration step $t_k = k\tau$ $(k = 1, \ldots)$ we use the iterative scheme

$$(\psi^{s+1/2} - \psi^s)/0.5\tau = \lambda_s(\Lambda_1\psi^{s+1/2} + \Lambda_2\psi^s + \omega^{s+1/2}),$$

$$(\psi^{s+1} - \psi^{s+1/2})/0.5\tau = \lambda_s(\Lambda_1\psi^{s+1/2} + \Lambda_2\psi^{s+1} + \omega^{s+1/2}),$$

where λ_s is an iteration parameter.

The method of cyclic sweep is used to find $T^{k+1/2}$, $\omega^{k+1/2}$, and ψ^{s+1}, and the so-called method of parametric sweep proposed by Voyevodin [6] is used to find ω^{k+1}, $\psi^{s+1/2}$. In accordance with [6], we write $\omega_{n,m} = P_{n,m}\omega_{N+1,m} + Q_{n,m}\omega_{1,m} + R_{n,m}$ and $\psi_{n,m} = \bar{P}_{n,m}\omega_{N+1,m} + \bar{Q}_{n,m}\omega_{1,m} + \bar{R}_{n,m}$.

4. Results of Numerical Analysis. Calculations are carried out on 21×21 and 41×41 grids for silicon, glycerin, or glass. The inside radius is $R_1 = 0.1$ cm ($R_1 = 0.5$ cm for some variants), and the outside radius is $R_2 = 1.1$ cm. Nondimensional parameters are given in Table 1.

When the capillary number Ca varies within the range of $10^{-5} \leqslant \mathrm{Ca} \leqslant 10^{-2}$ and $\gamma \sim 10^{-1}$ g/(sec$^2\cdot$ K) (see, for example, [7]), the calculations by the two models give only some quantitative differences in the flow characteristics. Figure 1 shows velocity fields and isotherms for glycerin at $\mathrm{Pr} = 10^4$ and $\mathrm{Ma} = 3 \cdot 10^2$ $(\mathrm{Re} = 3 \cdot 10^{-2})$.

The calculations have shown that the velocities calculated by the NM are approximately 20% higher than the velocities calculated by the OBM (the absolute values are compared).

The isotherms for glass and especially for silicon are less deformed and are similar in shape to the isotherms in the calculations of convective flows in domains with fixed boundaries [4]. Figure 2 shows velocity

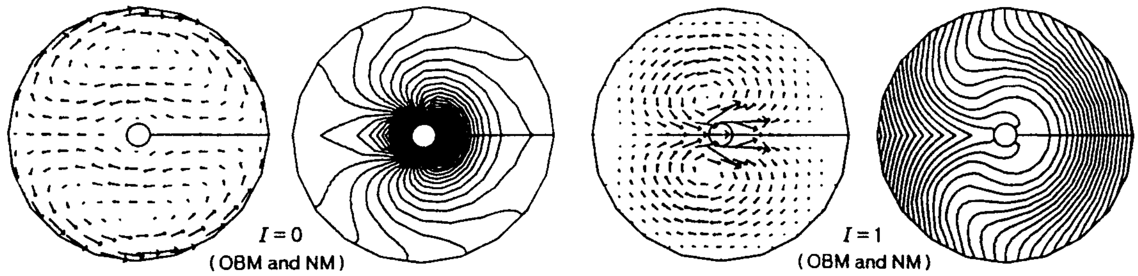

Fig. 1

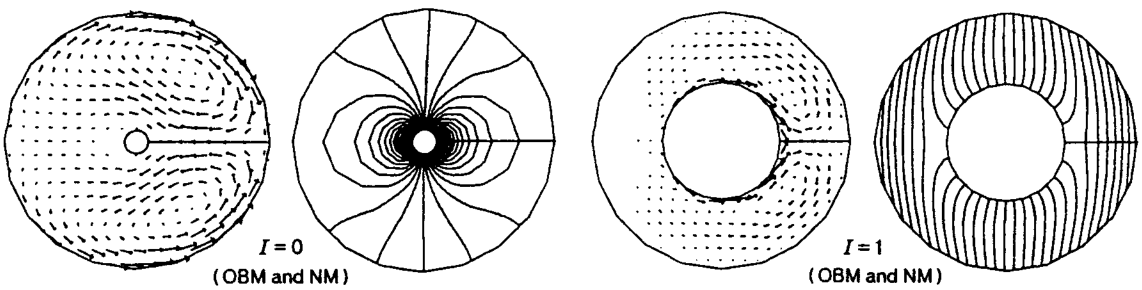

Fig. 2

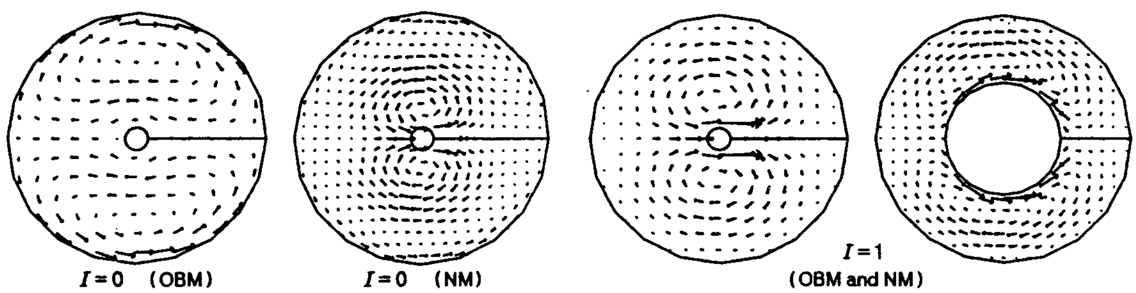

Fig. 3

fields and isotherms for silicon at $\mathrm{Pr} = 4\cdot 10^{-3}$ and $\mathrm{Ma} = 1$ ($\mathrm{Re} = 2.5\cdot 10^{2}$). The centers of vortices are shifted to the right.

The two-vortex structure of the velocity fields is characteristic of all cases, with some displacement of the centers of vortices to the left for glycerin.

There are some quantitative and qualitative differences between the results obtained by the two models at $10^{-5} \leqslant \mathrm{Ca} \leqslant 10^{-4}$ and $\gamma \sim 10^{-3}$ and 10^{-4} g/(sec$^2\cdot$ K). The parameters for numerical investigation are given in Table 2.

Figure 3 shows the velocity fields at $\mathrm{Pr} = 10^{4}$ and $\mathrm{Ma} = 1$ ($\mathrm{Re} = 10^{-4}$) which were calculated by the two models. For glycerin, in the case of $I = 0$ (the outer boundary is free), NM gives a two-vortex structure in each of the semicircular domains. For $I = 1$, either models give qualitatively the same flow pattern with only some quantitative differences.

It should be noted that the problem of convection stability in domains with free boundaries is of considerable interest (see, for example, [8]). The calculation results presented in [8] show that the instability can manifest itself at Re and Ma values greater than those of the present paper.

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