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EFFECT OF THERMAL DIFFUSION ON FREE CONVECTION OF A BINARY MIXTURE IN A CAVITY WITH A SQUARE CROSS-SECTION

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It is well known that the phenomenon of thermal diffusion can greatly affect the convective stability of a binary mixture consisting of nonreacting components [1]. Convective stability of equilibrium in a liquid binary mixture in a planar horizontal layer was studied in [2-9]. In [3-7], a hysteresis loop was obtained in Benard's problem for a two-component fluid and in [3-5] this problem was also studied experimentally. The effect of thermal diffusion on the convective stability of equilibrium and convective heat and mass transfer in a vertical gap was studied in [1, 10, 11]. In [12], the effect of thermal diffusion on heat transfer through a boundary layer was studied theoretically and experimentally. Free convection of a binary fluid mixture in an inclined rectangular cavity was investigated in [13].

In this paper, we study numerically free convection of a binary mixture in a square horizontal cylinder taking into account thermal diffusion. We examine lateral heating. It is assumed that thermal diffusion is the only reason for the appearance of a concentration inhomogeneity. The investigation is carried out for gas mixtures and aqueous solutions of salts. It is shown that in the presence of weak convection the normal thermal diffusion can double the convective velocity, while anamolous thermal diffusion can decrease it. For Rayleigh numbers of the order of 10^3, a vertical component appears in the concentration gradient at the center of the cavity. For anamalous thermal diffusion, it turns out that the maximum value of the stream function is not a unique function of the Rayleigh number (hysteresis is observed). For Rayleigh numbers exceeding 10^4, the effect of thermal diffusion on convective motion can be neglected.

We will examine an infinite square horizontal cylinder with height a, filled with a binary fluid mixture. The lateral boundaries are impenetrable and have different temperatures T_1 and T_2. The upper and lower boundaries are also impenetrable to matter and have a linear temperature distribution. If there is no convection in the cavity, then the concentration field arising as a result of the Soret effect is nearly linear [14, 15]. The maximum concentration differentials are very small [11], so that we will neglect energy flow caused by the inhomogeneity of the mixture. The Soret coefficient is assumed to be constant. The system of dimensionless equations describing two dimensional motion has the form [1, 16]

$$\frac{\partial\varphi}{\partial t}+\frac{\partial\psi}{\partial x}\frac{\partial\varphi}{\partial y}-\frac{\partial\psi}{\partial y}\frac{\partial\varphi}{\partial x}=\Delta\varphi+\mathrm{Gr}\left(\frac{\partial T}{\partial x}+\varepsilon\frac{\partial C}{\partial x}\right),$$

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$$\begin{gathered}\frac{\partial C}{\partial t}+\frac{\partial\psi}{\partial x}\frac{\partial C}{\partial y}-\frac{\partial\psi}{\partial y}\frac{\partial C}{\partial x}=\frac{1}{\mathrm{Sc}}(\Delta T+\Delta C),\\ \frac{\partial T}{\partial t}+\frac{\partial\psi}{\partial x}\frac{\partial T}{\partial y}-\frac{\partial\psi}{\partial y}\frac{\partial T}{\partial x}=\frac{1}{\mathrm{Pr}}\Delta T,\quad \Delta\psi=-\varphi,\end{gathered}\tag{1}$$

where ψ is the stream function; φ is the vorticity; T is the temperature; C is the concentration of the heavy components; $\mathrm{Pr} = \nu/\chi$ is Prandtl's number; $\mathrm{Sc} = \nu/D$ is Schmidt's number; $\mathrm{Gr} = g\beta_1(T_2 - T_1)a^3/\nu^2$ is Grashoff's number; $\varepsilon = \alpha\beta_2/\beta_1$ is the dimensionless thermal diffusion parameter; β_1, ν, χ, and D are the coefficients of thermal expansion, kinetic viscosity, thermal conductivity, and diffusion, respectively; $\alpha = k_0/T_0$ is the coefficient of thermal diffusion; k_0 is the thermal diffusion ratio; T_0 is the average temperature over the volume of the cavity; $\beta_2 = (1/\rho)(\partial\rho/\partial T)$; ρ is the density of the mixture.

In order to put the equations into dimensionless form, the following quantities were used as scales; a is the length scale; a^2/ν is the time scale; ν is the scale for the stream function; $(T_2 - T_1)$ is the temperature scale; and $\alpha(T_2 - T_1)$ is the concentration scale.

If all boundaries are solid and impenetrable to matter, then the boundary conditions have the form

$$\begin{gathered}\psi=\frac{\partial\psi}{\partial x}=0,\quad \frac{\partial T}{\partial x}+\frac{\partial C}{\partial x}=0,\quad \begin{cases}T=0 & \text{for}\quad x=0,\\ T=1 & \text{for}\quad x=1,\end{cases}\\ \psi=\frac{\partial\psi}{\partial y}=0,\quad \frac{\partial T}{\partial y}+\frac{\partial C}{\partial y}=0,\quad T=x\quad \text{for}\quad y=0,\ y=1.\end{gathered}\tag{2}$$

The system of equations (1) with boundary conditions (2) was solved numerically. An explicit finite difference scheme was used [17-21]. A uniform grid was introduced in the region $0 \le x \le 1$ and $0 \le y \le 1$

$$\begin{gathered}x_i=ih_1,\ i=0,\ 1,\ 2,\ \ldots,\ M,\ h_1=1/M,\\ y_k=kh_2,\ k=0,\ 1,\ 2,\ \ldots,\ K,\ h_2=1/K\end{gathered}$$

and the discrete step in time is $\tau = h^2(4 + \omega\psi_0)$, where h is the smallest coordinate step; ω is a parameter that is determined experimentally from the condition that the scheme be stable; ψ_0 is the maximum value of the stream function at each time step. Most of the calculations were carried out for M = 15, K = 15, and $\omega = 1, 2$. The spatial derivatives were replaced by central differences. In formulating the boundary conditions for the vorticity, we used Thom's equations [20]. Poisson's equation for the stream function was solved by the method of successive under-relaxation. The accuracy of the calculations was monitored by comparing the solutions on different grids. Some calculations were carried out additionally on 11 × 11 and 17 × 17 grids.

The linear temperature field $T_{ik} = ih_1$ and the zero field for the stream function $\psi_{ik} = 0$ were given as initial conditions. Two initial conditions were used for the concentration: either a linear field $C_{ik} = 1 - ih_1$ or a uniform field $C_{ik} = 0.5$. In some cases, the stationary state obtained in the calculations was used as an initial condition for determining the new stationary state, corresponding to other values of the parameters, for example, for higher Rayleigh number. Stationary motion was usually attained through damping of oscillations. The stabilization time of the stationary solution is determined by the initial state and by the dimensionless parameters: for parameters corresponding to gas mixtures, this time was 0.2-1.0 units.

The maximum value of the stream function was used as a characteristic of the intensity of convective motion, while Nusselt's number Nu was used as a characteristic of the intensity of heat transfer through the cavity, i.e., the dimensionless heat flow:

$$\mathrm{Nu}=\int_{\Gamma}\frac{\partial T}{\partial n}\,dl.$$

Here, $\partial T/\partial n$ is the normal component of the temperature gradient on the boundary of the cavity, while the integration is carried out over the region of the boundary in which the heat flux density has the same sign. In the absence of convection, Nu = 1.0.

The effect of thermal diffusion on convective motion was studied in greatest detail for gas mixtures with Pr = 1, Sc = 1-2. Numerical experiments were carried out for Rayleigh numbers $10 \le \mathrm{Ra} \le 10^5$ (Ra = GrPr). In the region $\mathrm{Ra} \le 10^3$, the maximum value of the stream function ψ_0 and of the Nusselt's numbers Nu depends linearly on the parameter $\mu = (1 + \varepsilon)\,\mathrm{Ra}$:

$$\psi_0 = A\mu,\ \mathrm{Nu} = 1 + B\mu.$$

The constants $A = 1.32 \cdot 10^{-3}$ and $B = 3.02 \cdot 10^{-4}$ turn out to be the same as in the case of a single-component fluid, studied previously in [19, 21]. Thus, in the region of Rayleigh numbers indicated above the intensity of

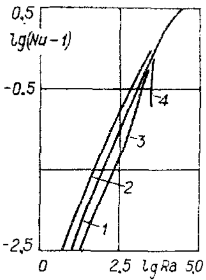

Fig. 1

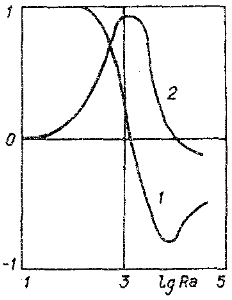

Fig. 2

convective motion turns out to be a factor of $(1 + \varepsilon)$ greater than for a single-component fluid. The structure of the flows, obtained for different Ra, ε, but with the same value of μ, is the same.

The dependence of the Nusselt number on the Rayleigh number for Pr = 1 and Sc = 1 is shown in Fig. 1 ($\varepsilon = 0, 1, -0.5$, and -1 for curves 1-4, respectively), from which it is evident that when the Rayleigh number increases in the region $\mathrm{Ra} \gtrsim 10^3$, the effect of the thermal diffusion parameter ε on the heat transfer intensity decreases and for $\mathrm{Ra} \gtrsim 10^4$ thermal diffusion does not affect heat transfer. The temperature field, in this case, has the same form as in the case of a single-component fluid. The dependence of the maximum value of the stream function ψ_0 on the Rayleigh number has the same form. For $\mathrm{Ra} \lesssim 10^2$, the distribution of temperature and concentration in the cavity is practically linear. In the region $\mathrm{Ra} \gtrsim 10^2$, appreciable distortions appear in the concentration field. Figure 2 shows the dependence of the vertical and horizontal components of the concentration gradient ($\partial C/\partial y$ and $\partial C/\partial x$ in curves 2 and 1, respectively) at the center of the cavity on Rayleigh's number for Pr = 1, Sc = 1, and $\varepsilon = 0.3$. The concentration gradient at the center of the cavity, having at first a horizontal orientation, begins to turn as a result of an increase in the vertical component and a decrease in the horizontal component. For $\mathrm{Ra} \sim 10^3$, the concentration gradient at the center of the cavity is almost vertical. It continues to rotate in the same direction as the Rayleigh number increases and can have an orientation opposite to the initial orientation.

The effect described is a result of the close interaction of convective motion, the usual diffusion, and thermal diffusion. It is reminiscent of the appearance of a vertical temperature differential and temperature stratification with convection of a single-component fluid in a closed region, studied previously in [22-24], but differs from the latter by a more complicated mechanism leading to its appearance. In contrast to concentration stratification, in alloys of liquid metals, arising with isogradient crystallization [25], the effect being examined is impossible in the absence of thermal diffusion. We recall that thermal diffusion in this paper is assumed to be the only reason for the appearance of concentration gradients.

The case of anomalous thermal diffusion with $\varepsilon \approx -1$ is of special interest. The dimensionless thermal diffusion parameter ε determines the ratio of buoyancy forces, caused by a perturbation of the concentration, to buoyancy forces caused by a temperature perturbation. A negative sign for the parameter ε shows that these forces have opposite orientations. In this connection, it turns out that mechanical equilibrium can exist for $\varepsilon = -1.0$. The well-known condition for mechanical equilibrium of a binary mixture [1] $(\beta_1 \nabla T + \beta_2 \nabla C) \cdot \gamma$ is satisfied in this case automatically, since $\beta_1 \nabla T + \beta_2 \nabla C = 0$. The density gradient, determined by temperature and concentration fields, equals zero. The direction of the temperature gradient can be arbitrary. In particular, mechanical equilibrium in a binary mixture is possible with lateral heating. In a single-component fluid, as is well known, mechanical equilibrium is possible only with strictly vertical temperature gradients [1]. With lateral heating, a binary mixture with $\varepsilon = -1.0$ can be in an equilibrium state until the diffusion of heat and mass smooths out density fluctuations. With intense heating, mechanical equilibrium becomes unstable.

Figure 3 shows the dependence of the Nusselt number on the Rayleigh number for gas mixtures with Pr = 1, Sc = 1, and $\varepsilon = -1.0$. For $\mathrm{Ra} < \mathrm{Ra}_1$, mechanical equilibrium is stable relative to both small and finite amplitude perturbations. (The stability of equilibrium was checked by introducing a vorticity at the center of the cavity with an amplitude corresponding to developed convective motion.) When Rayleigh numbers $\mathrm{Ra} \gtrsim \mathrm{Ra}_2 \approx 7500$ are attained, the equilibrium becomes unstable relative to small perturbations and convection suddenly appears with a finite amplitude. A decrease in Rayleigh's number leads to a decrease in heat transfer. For $\mathrm{Ra}_1 \approx 2700$, heat transfer drops sharply to zero. Thus, hysteresis, related to the possibility of exciting stationary convective motion in the subcritical region $(\mathrm{Ra}_1 < \mathrm{Ra} < \mathrm{Ra}_2)$ by introducing finite amplitude perturbations, occurs. Numerical experiments, carried out for gas mixtures with Sc = 2 and $\varepsilon = -1.0$, gave similar results. We note that in a flat horizontal layer of a binary mixture heated from below, the dependence of the Nusselt number on the Rayleigh number also exhibits a hysteresis loop [3-7].

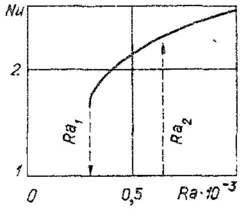

Fig. 3

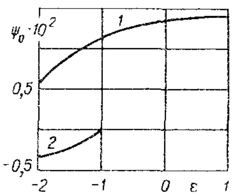

Fig. 4

Thermal diffusion convection was also studied for aqueous solutions of salts with Pr = 5 and Sc = 500. The large values of Pr and Sc, characteristic for fluids, lead to a large increase in machine time necessary for obtaining a stationary solution. For this reason, in order to conserve machine time, we change the time scale in solving the equations of thermal conductivity and diffusion. Control experiments showed that a change in the time scale permits obtaining rapidly a stationary solution and does not affect the final results. However, in studying the stability of motion, this method leads to large distortions of the results. For this reason, the stability of the solutions obtained was not studied.

In the case of anomalous thermal diffusion in fluid mixtures, two stationary solutions, differing by their intensity and the orientation of the convection and concentration fields, can also exist. As an example, Fig. 4 shows the dependence of the amplitude of the stream function on the dimensionless thermal diffusion parameter ε (Gr = 10). For such a Grashoff number, the intensity of motion is so low that the temperature field remains practically undistorted. Curve 1 corresponds to convective motion with the usual direction of circulation. The liquid rises at the heated wall and drops at the cold wall. The intensity of this motion decreases with decreasing ε. The concentration gradient at the center of the cavity decreases by an order of magnitude. Curve 2 corresponds to motion with oppositely directed circulation. The fluid rises at the cold wall and drops at the hot wall. The concentration gradient at the center of the cavity turns by some angle (up to 40-60°). The magnitude of the concentration gradient varies insignificantly. The existence of such motion was discovered, at least, for $\varepsilon \leq -1$.

Both for positive as well as for negative values of the thermal diffusion parameter ε, convective motion had a structure similar to the structure of the motion of a single component fluid with corresponding Rayleigh numbers. Since in the present work the investigations were carried out in the region $Ra < 10^5$, double-vortex motion, discovered previously in [19], was not observed. The maximum value of the stream function was always found at the center of the cavity. Thermal diffusion was not observed to have a large effect on the structure of the motion.

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MODEL OF A NONEQUILIBRIUM TWO-PHASE ZONE TAKING INTO ACCOUNT CONVECTION OF A BINARY MELT

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A mathematical model of a two-phase dendrite zone was constructed in [1, 2] for nonequilibrium crystallization of a binary melt. In this case, the change in the density of the melt in the phase transformation process was neglected and the melt was assumed to be stationary. It is evident that when a crystal grows, as a result of settling phenomena, a flow of the liquid phase, oriented toward the crystal, must exist in the melt. This effect was examined in [3, 4] for crystallization of pure metals. It is shown therein that the flows of the melt arising affect the temperature and pressure field in the liquid phase. In the process of nonequilibrium crystallization of a binary melt, these flows will also affect the distribution of the admixture in the liquid phase and, therefore, the structure of diffusion overcooling as well. Since the kinetics of the growth and morphology of dendrites in the two-phase zone are determined by overcooling of the melt, this effect will affect the development of the two-phase zone as a whole, as well as the nature of the chemical inhomogeneity and formation of porosity in the ingot.

In what follows, based on phenomenological assumptions, we formulate a mathematical model of heat and mass transfer processes in the two-phase zone of a solidifying binary alloy taking into account the kinetics of growth of dendrites and the density discontinuity along the phase separation surface.

Let us examine directed crystallization of a binary melt in the presence of a two-phase zone. The scheme of the physical model is illustrated in Fig. 1. We assume that the two-phase zone consists of homogeneous dendrites with a column ($\nu = 1$) or plate ($\nu = 0$) form, while their growth velocity along the normal to the surface of the crystal is an exponential function of the local overcooling ΔT:

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