CONCENTRATION CONVECTION IN A SOLIDIFYING MELT

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UDC 536.25:620.186.2

Up to the present time, one of the main reasons for the mixing of the liquid core of a hardening melt has been considered to be thermal gravitational convection. At the same time, it is to be expected that the concentrational inhomogeneity arising during the process of solidification, being nonidentical in its composition, will also have a considerable effect on the process of the mixing of the liquid core of a hardening melt.

For the construction of a mathematical model of concentration convection, a rectangular region with transverse cross-sectional dimensions $L_1 \times L_2$, semiinfinite along a horizontal coordinate and normal to the plane of the cross section, was considered. Along the horizontal dimension L_1, the coordinate $\eta_1(\xi_1)$ is plotted and along the vertical dimension L_2 the coordinate $\eta_2(\xi_2)$.

The region is filled with a melt having an initial impurity content C_0. The initial temperature of the melt T_0 is essentially close to the crystallization temperature T_c. The initial state is a state of rest, with a uniform distribution of the impurity and the temperature over a cross section of the region.

As the boundary of the solidification we take a flat surface, directly separating the solid and liquid phases. The law of the forward motion of the boundary of the phase transition is taken from the classical solution of the Stefan problem, in the form of the law of the "square root"

$$\varepsilon_1 = l_1 - \alpha\sqrt{F_0},\ \varepsilon_2 = l_2 - \alpha\sqrt{F_0},\ R_1 = R_2 = \alpha\sqrt{F_0},$$

where $l_1 = L_1/x_0$ is the relative width of the plane; $l_2 = L_2/x_0$ is the relative height of the cavity of the crystallizer; x_0 is the characteristic dimension of the region; $F_0 = D\tau/x_0^2$ is the dimensionless time; D is the diffusion coefficient of the impurity in the liquid phase; α is the solidification coefficient.

Such an approach to the determination of the position with time of the boundaries of the phase transition is justified. A conjugate solution [1], during the course of which the motion of the boundary of the phase transition was determined, showed that there is no substantial deviation from the law of the "square root"; the solution of the problem itself and the program are complicated considerably and the calculating time increases.

At a moment of time differing from zero ($t > 0$), the temperature of the region boundaries drops jumpwise to the crystallization temperature of the melt. The temperature inhomogeneity arising under these circumstances as a result of the closeness of T_0 and T_c is assumed to be insufficient for the origin and development of a thermal convective motion in the melt. This follows from an evaluation of the relative role of thermal and concentration convection: A comparison of the dimensionless Gr and Ar_0 numbers show that, with small degrees of superheating, $Gr/Ar_0 \sim 10^{-3} \ll 1$, where $Gr = g\beta(T_0 - T_c)x_0^3/\nu^2$ is the Grashof number; $Ar_0 = \gamma g C_0 x_0^3/\nu^2$ is the modified Archimedes number; $\nu = 1.27 \cdot 10^{-6}$ m^2/sec is the coefficient of kinematic viscosity; $\beta = 0.17 \cdot 10^{-3}$ deg^{-1} is the coefficient of volumetric expansion; g is the acceleration due to gravity; γ is a coefficient characterizing the relative change in the density as a function of the concentration,

$$\gamma = \frac{1}{\rho}\frac{\Delta\rho}{\Delta C} \approx 0.25, \quad C_0 = 0.03\%.$$

The difference in the solubility of the impurity in the solid and liquid phases brings about three-dimensional inhomogeneity of the concentration field. Under these conditions with determined concentration gradients in the liquid core existing in a gravitational field, a convective motion arises, whose direction is determined by the ratio of the density of the impurity and the density of the mother melt.

Determining the characteristic velocity and the characteristic pressure difference, respectively, by the expressions $u_0 = \nu/x_0$, $p_{max} - p_{min} = \rho_0 u_0^2$, where $p_{max} - p_{min}$ is the characteristic pressure difference and ρ_0 is the density of the melt, we write the equation of motion

Donetsk. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 6, pp. 98-103, November-December, 1977. Original article submitted November 11, 1976.

0021-8944/77/1806-0812$07.50

$$\frac{\partial \mathbf{V}}{\partial F_0} + (\mathbf{V}\nabla) = -\nabla\pi + \mathrm{Sm}\,\Delta\mathbf{V} \pm \mathbf{I}_g\,\mathrm{Sm}^2\,\mathrm{Ar}_0\,\delta S, \tag{1}$$

where $\delta S = S_b - S$ for every moment of time is defined as the difference between the concentrations at points of the boundaries of the phase transition and points located at the corresponding lines of the grid, starting from which the concentration gradient can be neglected (as such points there were taken points at which the concentration is less than that at the preceding points by 0.01): $\pi = p/(p_{max} - p_{min})$ is the dimensionless pressure; $Sm = \nu/D$ is the Schmidt number; I_g is a unit vector, coinciding with the direction of g.

The equation of diffusion

$$\partial S/\partial F_0 + (\mathbf{V}\nabla)S = \Delta S$$

($S = C/C_0$ is the dimensionless concentration), the equation of continuity

$$\nabla\mathbf{V} = 0.$$

The given system is completed by the following initial and boundary conditions:

$$\mathbf{V}|_{F_0=0} = 0,\ S|_{F_0=0} = 0,\quad V_1|_{\eta_1=\varepsilon_1} = V_1|_{\eta_1=R_1} = V_1|_{\eta_2=\varepsilon_2} = V_1|_{\eta_2=R_2} = 0,$$
$$V_2|_{\eta_1=\varepsilon_1} = V_2|_{\eta_1=R_1} = V_2|_{\eta_2=\varepsilon_2} = V_2|_{\eta_2=R_2} = 0,$$

where $V_1 = u_1/u_0$, $V_2 = u_2/u_0$ are the dimensionless components of the velocity along the axes η_1 and η_2, respectively.

The boundary conditions for the concentration are written at each boundary of the region; here the difference in the impurity solubility in the solid and liquid phases is taken into account by the equilibrium coefficient of the impurity redistribution k; the impurity diffusion in the solid phase is neglected in comparison with the liquid phase:

$$-\frac{\partial S}{\partial \eta_1}\Big|_{\eta_1=\varepsilon_1} = \varepsilon_1'(1-k)\,S|_{\eta_1=\varepsilon_1},\quad -\frac{\partial S}{\partial \eta_1}\Big|_{\eta_1=R_1} = R_1'(1-k)\,S|_{\eta_1=R_1},$$
$$-\frac{\partial S}{\partial \eta_2}\Big|_{\eta_2=R_2} = R_1'(1-k)\,S|_{\eta_2=R_2},\quad -\frac{\partial S}{\partial \eta_2}\Big|_{\eta_2=\varepsilon_2} = \varepsilon_2'(1-k)\,S|_{\eta_2=\varepsilon_2},$$

where $\eta_1 = x_1/u_0$, $\eta_2 = x_2/x_0$ are dimensionless coordinates; R_1', ε_1', R_2', ε_2', are the velocities of the motion of the lateral, upper, and lower boundaries.

The problem was solved by the method of finite differences [2], using the integrointerpolational method and the method of fractional spacings [3].

For the subsequent transformation the following were introduced: the stream function ψ; the curl of the velocity φ; and the new variables ζ_1 and ζ_2, mapping a rectangular region with movable boundaries on the region of a unit square, so that, during the time of the solidification process, $0 \le \zeta_1 \le 1$, $0 \le \zeta_2 \le 1$, where

$$\zeta_1 = (\eta_1 - R_1)/(\varepsilon_1 - R_1);\ \zeta_2 = (\eta_2 - R_2)/(\varepsilon_2 - R_2).$$

The uniform coordinate and time grids were chosen in the form

$$\omega_h = \{\zeta_1 = ih,\ \zeta_2 = mh,\ h = 1/I = 1/M > 0;\ i = 0, 1, 2, \ldots, I;$$
$$m = 0, 1, 2, \ldots, M\},$$

$$F_{0n} = \left\{F_0 = \sum_{\nu=0}^{n}\tau_\nu,\quad \tau_\nu = A\frac{n^2}{4},\quad 0 < A < 1\right\}.$$

The coordinate grid used in the calculation had a dimension $\omega_h = 32 \times 32$. The algorithm for calculation of the system of the equations of motion and mass transfer corresponded to [4]. The numerical solution of the system was carried out on a Dnepr-21 digital computer.

The specific weight of the impurity was assumed to be greater than the specific weight of the mother melt; therefore, the term $\mathrm{Sm}^2\mathrm{Ar}_0\delta S$ in Eq. (1) was taken as positive.

An investigation of concentrational gravitational convection was made for the Archimedes numbers $\mathrm{Ar}_0 = 0.2 \cdot 10^n$ ($n = 7, 8, 9$). In view of the fact that the character of the convective motion is, in general, conserved for all the above Archimedes numbers, a detailed analysis of convective motion was made for the number

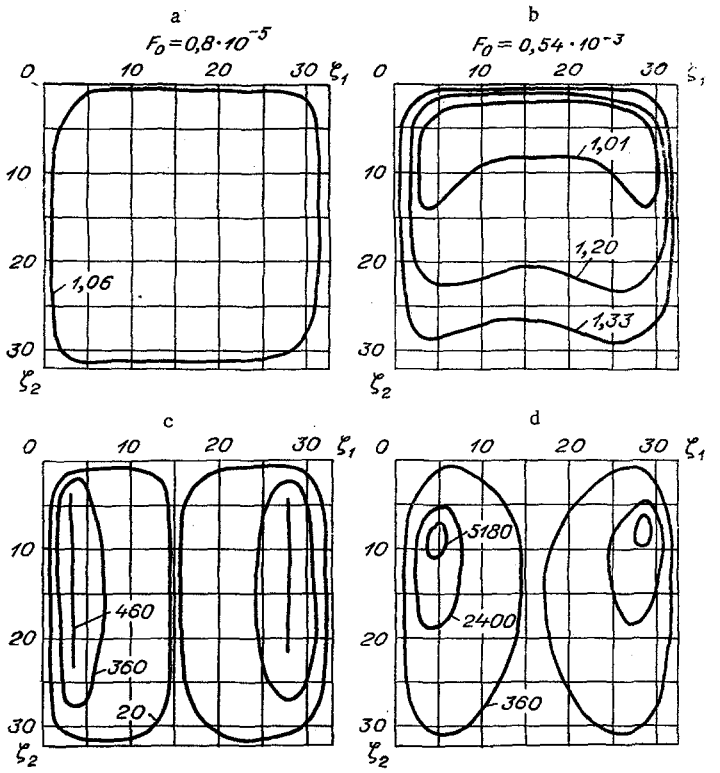

Fig. 1

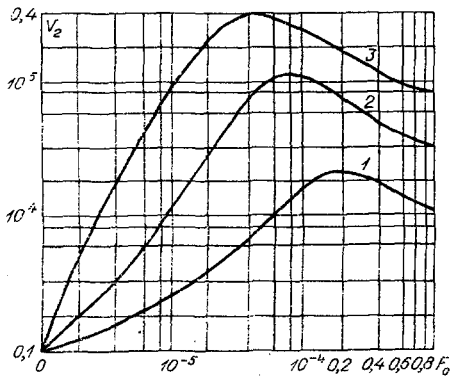

Fig. 2

$Ar_0 = 0.2 \cdot 10^8$, while, for the numbers $Ar_0 = 0.2 \cdot 10^n$ (n = 7, 9), only a few singularities were investigated. The problem was solved with the following parameters:

$$x_0 = 600 \text{ mm}, \ \omega_h = 32 \times 32, \ \alpha = 10, \ k = 0.5.$$

The geometry for which the calculation was made was such that $l_2/l_1 = 3$. The relative error of the calculation was determined during the course of a numerical experiment and, for a coordinate grid with a dimension of 32×32, did not exceed 5%.

An analysis of the results of the calculation shows that, at a moment of time differing from zero, the excess impurity is displaced out of the solid phase to the phase interface. This brings about the development of a certain concentration inhomogeneity at the boundary of the phase transition, characterized by a maximal concentration gradient (Fig. 1a, b, $F_0 = 0.8 \cdot 10^{-5}$, $0.54 \cdot 10^{-3}$, respectively).

The melt along the boundary of the phase transition, enriched in the impurity, sinks down to the bottom part of the liquid core, by the same token setting into motion, toward the upper boundary of the cavity of the crystallizer, the melt which is enriched in the impurity to a lesser degree, due to its greater distance from the boundary of the phase transition. As a result of this, in the liquid core of the solidifying melt, as in the

case of thermal gravitational convection [5], there arise two vortices of the velocity, symmetrical with respect to the vertical axis of symmetry of the crystallizer cavity and asymmetrical with respect to the horizontal plane passing through the middle of the axis $O\zeta_2$ (Fig. 1c, d, $F_0 = 0.8 \cdot 10^{-5}$; $0.54 \cdot 10^{-3}$, respectively). The results of the calculation show that, in the initial period, the zone of "descending" flows is narrower than the zone of "ascending" flows. With development of the motion, the zone of "descending" flows expands and the zone of "ascending" flows contracts. Under these circumstances, near the limit of the phase transition, the component of the velocity V_2 attains a maximal value.

The character of the time distribution of the maximal value of the component of the velocity of the convective motion V_2 makes it possible to divide the whole process of convective motion into two periods: a period of the acceleration of the liquid core of the hardening melt to a maximal value of the velocity and a period of slow decrease in the velocity; the first period is considerably shorter than the second (Fig. 2, curve 2, $Ar_0 = 0.2 \cdot 10^8$). Such a distribution of the velocity is obviously a consequence of the fact that, in an interval of time corresponding to the first period, there is a restructuring of the concentration field, as a result of which in the liquid core of the hardening melt greater concentration gradients arise, bringing about a rise in the rate of increase of the convective motion.

The process of a slow decrease in the velocity of the convective motion against the background of an overall increase in the concentration of the impurity in the liquid core of the hardening melt is obviously explained by the fact that, with a comparatively slow increase in the level of the impurity in the liquid core, the level of its concentration inhomogeneity decreases at approximately the same rate.

The total duration of the convective motion is due to the presence of concentration inhomogeneity, which exists up to the end of the hardening process. This explains the rather high rate of convective motion practically up to complete solidification of the ingot; here the difference between the maximal and minimal values of the velocity is approximately 10%. An increase in the Ar_0 number has a considerable effect on increasing the level of the rate of development of convective motion. Thus, even with a value of the Archimedes number $Ar_0 = 0.2 \cdot 10^9$ (see Fig. 2, curve 3), a concentration gradient arises in the melt, sufficient in value to bring the whole mass of the liquid core of the hardening melt into motion at a moment of time ($F_0 = 0.81 \cdot 10^{-5}$) practically coinciding with the start of the process. With an increase in the Ar_0 number, there is a rise in the value of the term of the equation of convective motion (1) $Sm^2 Ar \delta S$, an increase in which, even at the start of the development of the process, determines a level of the concentration inhomogeneity sufficient to bring the whole mass of the melt into motion. This also promotes a higher rate of development of the process of convective motion as a whole.

The shortening of the period of acceleration of the melt to a maximal value, noted in Fig. 2 (curve 3), is obviously explained by the above reason.

With a decrease in the Ar_0 number ($Ar_0 = 0.2 \cdot 10^7$), the maximal value of the rate of motion of concentrational convection decreases appreciably (see Fig. 2, curve 1). Under these circumstances, the period of acceleration of the melt to a maximal value of the velocity increases.

This is explained by the fact that, with a decrease in the Ar_0 number, there is a decrease in the value of the term $Sm^2 ar_0 \delta S$ of Eq. (1). This leads to a considerable lowering of the level of the concentration inhomogeneity, which is the reason for the slower development of all the above-described processes.

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