



Soviet-era science, translated into English

Reports of the Academy of Sciences of the USSR

1966

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Abstract

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Reports of the Academy of Sciences of the USSR
1966. Volume 168, No. 5

UDC 536.248.2

MATHEMATICAL PHYSICS

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ON THE INITIAL DIRECTION OF THE CRYSTALLIZATION PROCESS WHEN A PLATE IS IMMERSSED IN A MELT

(Presented by Academician A. A. Dorodnitsyn, 20 IX 1965)

Let an infinite plate of thickness $2l$, with melting temperature T and initial temperature T_0 , be immersed in a melt of temperature T_1 with crystallization temperature T . We shall assume that: a) $T_0 < T \leq T < T_1$; b) the melt is maintained in a state of intense stirring. A constant amount of heat q is prescribed (per unit surface area and unit time) as falling from the core of the melt onto the plate; c) the temperature in the boundary layer separating the core of the melt from the plate varies linearly in the direction normal to the surface of the plate; d) the coefficients of thermal expansion of the plate material in the solid and liquid phases and of the melt material in the solid phase are equal to zero; e) the solid and liquid phases of the plate material have the same density; and f) the phase-transition process proceeds reversibly, without superheating or supercooling. The heat in the liquid phase formed during melting of the plate is propagated by heat conduction, without convection.

Under these assumptions, the process of redistribution of temperatures and phase states in the system under consideration will be described by Fourier equations and Stefan conditions.

A priori, one may conceive of three possible initial paths of development of the process: a) crystallization of the melt and melting of the plate begin simultaneously, at the moment of its immersion; b) melting of the plate precedes crystallization of the melt; and c) crystallization of the melt precedes melting of the plate. Our task is to investigate along which of these paths the process will proceed in reality. In this connection we emphasize that the scheme under consideration is an idealization not realizable under natural conditions. Therefore, when speaking of the path along which the process will actually proceed, we have in mind the analysis of our idealized scheme, and only of it, without in any way assuming that the conclusions at which we arrive can be used to judge the real natural process. Nevertheless, we believe that elucidating the question

posed within the adopted idealization is of interest, since it clarifies the very formulation of the problem and indicates a way to analyze the process also in schematizations closer to reality.

Introduce dimensionless variables by putting

$$\begin{aligned}
 x &= \tilde{x}/l; & t &= \tilde{a}_1^2 \tilde{t}/l^2; & u &= (T - T)/(T_0 - T); \\
 \vartheta &= (T - T)/(T_0 - T); \\
 a_i^2 &= \tilde{a}_i^2/\tilde{a}_1^2; & k_i &= \tilde{k}_i/\tilde{k}_1; & \lambda_i &= k_3 a_i/k_i a_3;
 \end{aligned} \tag{1}$$

$$\delta_i = (1 - \lambda_i)/(1 + \lambda_i),$$

$$\beta_i = \tilde{k}_i(T_0 - T)/\tilde{\gamma}_i \tilde{\rho}_i \tilde{a}_1^2; \quad \mu_i = \tilde{k}_i(T_0 - T)/\tilde{\gamma}_i \tilde{\rho}_1 \tilde{a}_1^2; \quad \alpha_i = ql/\tilde{\gamma}_i \tilde{\rho}_i \tilde{a}_1^2.$$

Here the sign \sim denotes dimensional quantities; the index $i = 1, 2, 3$ refers respectively to the solid phase of the plate, its liquid phase, and the solid

phase of the material of the external melt; γ_i , ρ_i , k_i , and a_i^2 are the latent heat of the phase transition, the density, the coefficient of thermal conductivity, and the coefficient of thermal diffusivity of the i -th phase; T is the temperature at the point \tilde{x} at the instant \tilde{t} ; the quantities γ_i, \dots, a_i^2 are regarded as constants.

In the variables x , t , u , the initial stage of the process will, depending on its path, be described by the following conditions.

A. Crystallization of the melt and melting of the plate begin simultaneously.

$$\begin{aligned}
 a^2(x) \frac{\partial^2 u}{\partial x^2} &= \frac{\partial u}{\partial t}; & 0 < x < y(t); & & x \neq z(t); \\
 x &\neq 1; & t > 0;
 \end{aligned} \tag{2_1}$$

$$\begin{aligned}
 \frac{\partial u}{\partial x} \Big|_{x=0} &= 0; & u|_{x=z \pm 0} &= \vartheta; & u|_{x=y-0} &= 0; & t > 0; \\
 u|_{t=0} &= 1; & 0 < x < 1;
 \end{aligned} \tag{2_2}$$

$$u|_{x=1-0} = u|_{x=1+0}; \quad k_1 \frac{\partial u}{\partial x} \Big|_{x=1-0} = k_2 \frac{\partial u}{\partial x} \Big|_{x=1+0}; \quad t > 0; \tag{2_3}$$

$$\dot{z}(t) = \mu_1 \frac{\partial u}{\partial x} \Big|_{x=z-0} - \mu_2 \frac{\partial u}{\partial x} \Big|_{x=z+0}; \quad t > 0; \quad z(0) = 1; \quad (2_4)$$

$$\dot{y}(t) = \alpha_3 + \beta_3 \frac{\partial u}{\partial x} \Big|_{x=y(t)-0}; \quad t > 0; \quad y(0) = 1. \quad (2_5)$$

Here

$$\begin{aligned} a^2(x) &= a_i^2; \\ i &= 1 \text{ for } 0 < x < z(t); \quad i = 2 \text{ for } z(t) < x < 1; \\ i &= 3 \text{ for } 1 < x < y(t); \end{aligned} \quad (2_6)$$

$x = z(t)$ is the equation of the melting front of the plate, and $x = y(t)$ is the equation of the crystallization front of the melt.

B. Melting of the plate precedes crystallization of the melt.

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}; \quad 0 < x < z(t); \quad t > 0; \quad (3_1)$$

$$\frac{\partial u}{\partial x} \Big|_{x=0} = 0; \quad u|_{x=z(t)} = \vartheta; \quad t > 0; \quad u|_{t=0} = 1; \quad 0 < x < 1; \quad (3_2)$$

$$\dot{z}(t) = -\alpha_1 + \beta_1 \frac{\partial u}{\partial x} \Big|_{x=z(t)-0}; \quad t > 0; \quad z(0) = 1. \quad (3_3)$$

In accordance with the physical meaning of the problem, path B is possible if, in a neighborhood of $t = 0$, $z(t) < 1$.

C. Crystallization of the melt precedes melting of the plate.

$$a^2(x) \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}; \quad 0 < x < y(t); \quad t > 0; \quad x \neq 1; \quad (4_1)$$

$$\frac{\partial u}{\partial x} \Big|_{x=0} = 0; \quad u|_{x=y(t)} = 0; \quad t > 0; \quad u|_{t=0} = 1; \quad 0 < x < 1; \quad (4_2)$$

$$u|_{x=1-0} = u|_{x=1+0}; \quad k_1 \frac{\partial u}{\partial x} \Big|_{x=1-0} = k_3 \frac{\partial u}{\partial x} \Big|_{x=1+0}; \quad t > 0; \quad (4_3)$$

$$\dot{y}(t) = -\alpha_3 + \beta_3 \frac{\partial u}{\partial x} \Big|_{x=y(t)}; \quad y(0) = 1. \quad (4_4)$$

Here

$$a^2(x) = a_1^2 \text{ for } 0 < x < 1, \quad a^2(x) = a_3^2 \text{ for } 1 < x < y(t). \quad (4_5)$$

Along path C the process can proceed in the case when, in addition to conditions (4₁)-(4₄), the condition

$$u(1, t) > \vartheta; \quad t > 0 \quad (4_6)$$

is satisfied.

Let us first investigate path A. We shall use the notation

$$\frac{\partial u}{\partial x} \Big|_{x=z-0} = v_1(t); \quad \frac{\partial u}{\partial x} \Big|_{x=z+0} = v_2(t); \quad \frac{\partial u}{\partial x} \Big|_{x=y-0} = v_3(t);$$

$$\sqrt{t} v_i(t) = w_i(t) \quad (i = 1, 2, 3); \quad \lim_{t \rightarrow 0} \sqrt{t} \dot{z}(t) = -\gamma_1; \quad \lim_{t \rightarrow 0} \sqrt{t} \dot{y}(t) = \gamma_3; \quad (5)$$

$$\xi = \frac{\gamma_1}{a_2}; \quad \eta = \frac{\gamma_3}{a_3}; \quad A = \frac{a_2^2 \beta_3}{a_3^2 \mu_2} \frac{1}{\lambda_2}; \quad B = \frac{a_3^2 \mu_2}{a_2^2 \beta_3}.$$

Using the same methods for investigating the initial behavior of the system as those we applied earlier ^(1,2), we find that

$$w_1(0) = -\frac{1 - \vartheta}{\sqrt{\pi}} \frac{\exp(-a_2^2 \xi^2)}{\operatorname{erfc}(a_2 \xi)}; \quad (6_1)$$

$$w_2(0) = -\frac{\vartheta(1 - \delta_2)}{a_2 \sqrt{\pi}} \exp(-\xi^2) - w_2(0)[\operatorname{erf} \xi + \delta_2 \operatorname{erfc} \xi] + \\ + w_3(0)(1 - \delta_2) \frac{a_2}{a_3} \exp(\eta^2 - \xi^2) \operatorname{erfc} \eta; \quad (6_2)$$

$$w_3(0) = -\frac{\vartheta(1 + \delta_2)}{a_3 \sqrt{\pi}} \exp(-\eta^2) + w_2(0)(1 + \delta_2) \frac{a_2}{a_3} \exp(\xi^2 - \eta^2) \operatorname{erfc} \eta - \\ - w_3(0)[\operatorname{erf} \eta - \delta_2 \operatorname{erfc} \eta]. \quad (6_3)$$

At the same time, from (5), (2₄), and (2₅) it follows that

$$\xi = \frac{\mu^2}{a_2} w_2(0) - \frac{\mu_1}{a_2} w_1(0); \quad \eta = \frac{\beta_3}{a_3} w_3(0). \quad (6_4)$$

Eliminating $w_i(0)$ from the system (6_{*i*}) ($i = 1, \dots, 4$), we obtain

$$f_1(\eta) = f(\xi); \quad \varphi_1(\eta) = \varphi(\xi). \quad (7)$$

Here

$$\begin{aligned} \varphi_1(\eta) &= \eta \exp(\eta^2); & \varphi(\xi) &= A \exp(\xi^2) \left[\xi - \frac{\mu_1(1 - \vartheta) \exp(-a_2^2 \xi^2)}{a_2 \sqrt{\pi} \operatorname{erfc}(a_2 \xi)} \right]; \\ f_1(\eta) &= \varphi_1(\eta) \operatorname{erfc} \eta; & f(\xi) &= \varphi(\xi) (1 + \lambda_2 \operatorname{erf} \xi) + \frac{\vartheta \beta_3}{a_3^2 \sqrt{\pi}}; \end{aligned} \quad (8)$$

$$A = a_2^2 \beta_3 (a_3^2 \mu_2 \lambda_2)^{-1}.$$

Let η_1 and η_2 be the roots of the equations

$$\varphi_1(\eta_1) = \varphi(0); \quad f_1(\eta_2) = f(0). \quad (9)$$

Investigating the arrangement of the curves (7) and noting that, by assumption, $y(t) > 1$, $z(t) < 1$, and near $t = 0$

$$\operatorname{sgn} \dot{z}(t) = \operatorname{sgn}(-\xi); \quad \operatorname{sgn} \dot{y}(t) = \operatorname{sgn} \eta, \quad (10)$$

we easily find that development of the process along path A is possible if $f(0) < 0$, or if $0 \leq f(0) < 1/\sqrt{\pi}$ and simultaneously $\eta_2 < \eta_1$. Conversely, development of the process along path A is impossible if $f(0) \geq 1/\sqrt{\pi}$, or if $0 \leq f(0) < 1/\sqrt{\pi}$ and simultaneously $\eta_1 < \eta_2$.

Let us note that the formulated conditions for the possibility of development of the process along path A have been obtained only as necessary conditions. However, using the methods developed in ^(2,3), one can show that, when the necessary conditions found above for the possibility of development of the process along path A are satisfied, the solution of problem (2₁)–(2₆) exists and is unique. Thus, the conditions found are not only necessary but also sufficient conditions for the possibility of the process following path A.

We now examine path B. It is easy to show that in this case

$$\lim_{t \rightarrow 0} \frac{\partial}{\partial x} u \Big|_{x=z(t)} = -\infty. \quad (11)$$

Since $\beta_1 < 0$, it follows from this, by virtue of (3₃), that $\lim_{t \rightarrow 0} \dot{z} = +\infty$. Thus, development of the process along path B is impossible.

Consider, finally, path C. Note that, up to the notation, equations (4₁)—(4₅) coincide with the equations investigated in (2, 3). Thus, the solution of problem (4₁)—(4₅) exists and is unique. Therefore, in order to judge the possibility of development of the process along path C, it is only necessary to determine in which case condition (4₆) is satisfied. It is easy to show that

$$\lim_{t \rightarrow 0} u_1(1, t) = (1 + \delta_1) \left\{ 1 - \frac{1 - \operatorname{erf} \gamma_1}{1 + \frac{1}{\lambda_1} \operatorname{erf} \gamma_1} \right\} \equiv F, \quad (12)$$

where γ_1 is the root of the equation

$$\gamma_1 = -\frac{\beta_1 \exp(-\gamma_1^2)}{\lambda_1 a_2^2 \sqrt{\pi}} - \frac{\gamma_1}{\lambda_1} \operatorname{erf} \gamma_1. \quad (13)$$

Consequently, development of the process along path C is possible if $F > \vartheta$, and impossible if $F < \vartheta$.

It should be borne in mind that, when we speak of the “possibility” of development of the process along path A or C, we mean only the internal consistency of the equations of the problem, written under the assumption that the process develops along this path. On which path the process will in fact develop cannot, generally speaking, be said on the basis of the information obtained. Indeed, the values of the parameters determining the process may be such that the “possibility” conditions for paths A and C prove to be compatible. To see this, let us require that the inequality

$$\theta \equiv \frac{1 - \vartheta}{k_3} - \frac{\vartheta}{a_3} < 0 \quad (14)$$

be satisfied.

It is easy to verify that $\operatorname{sgn} f(0) = \operatorname{sgn} \theta$. Thus, when condition (14) is fulfilled, development of the process along path A is certainly possible. Let us now fix a ϑ satisfying condition (14), and suppose that $1 + \delta_1 > \vartheta$. Since F in (12) varies from zero for $\gamma_1 = 0$ to $1 + \delta_1$ as $\gamma_1 \rightarrow \infty$, we see that, under the condition $1 + \delta_1 > \vartheta$, there exists a $\gamma_1 > 0$ satisfying the requirement $F > \vartheta$. Fix such a γ_1 and determine β_1 from equation (13), which will ensure fulfillment of the condition for the possibility of the process following path C.

Thus, to determine the actual initial direction of development of the process, information additional to that already obtained may be required. This information cannot be extracted from the equations for the process following paths A or C without invoking additional physical principles, which lies beyond the scope of the present investigation.*

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Received
13 IX 1965

CITED LITERATURE

- ¹ L. I. Rubinshtein, DAN, **62**, No. 6 (1948).
- ² L. I. Rubinshtein, DAN, **160**, No. 5 (1965).
- ³ L. I. Rubinshtein, DAN, **168**, No. 4 (1966).

* The question could be decided within the framework of the thermodynamics of irreversible processes. Apparently, the process should proceed along the path along which the rate of entropy increase is maximal. However, this question requires special study. In connection with this, let us note that the admissibility of applying thermodynamic principles to the question under investigation is unclear, since our description of phase-transition processes is based on the assumption of their reversibility, whereas any actually occurring process of formation of a new phase is impossible without preliminary supercooling or overheating of the system, and, therefore, the mathematical description of the process is inadequate to its physical nature.

Note: Figure translations are in progress. See original paper for figures.

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