NUMERICAL INVESTIGATION OF THE HEATING OF CONDENSED MEDIA BY VOLUME HEAT SOURCES

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One possible mechanism of action on materials involves the production of volume heat sources in them either by absorption of electromagnetic radiation or passage of an electric current. In both cases, the action is determined by distributed volume heat sources. As a result of the action of these sources there can arise in the material a region with a phase transition, and it is the development of this region that determines the change in the physical properties and the softening of the material. Examples of such action in practice are the action of solar radiation on ice and frozen soil [1-4] and of electromagnetic radiation on various materials [5, 6].

A characteristic feature of a phase transition in the presence of distributed volume heat sources is the existence of a finite isothermal transitional region [7], determined by the fact that the temperature in it has reached the phase transition point but the absorbed energy is still below the phase-transformation energy. In the general case a boundary of this region can be the boundary of discontinuity of the distribution of the internal energy [7, 8]. This problem was analyzed mathematically in [7], where it was proved that the generalized Stefan problem has a unique solution and the boundary conditions were established in different cases. Examples of the solution of problems of a phase transition with an isothermal zone are presented in [4, 5] and actual experimental data are presented in [1, 2].

In the present paper we investigate numerically — in a one-dimensional approximation within the generalized Stefan problem — the development of a region of phase transformation (melting) in a material under the action of distributed heat sources. The evolution of the isothermal region depends on the thermal regime, the thermophysical properties of the materials, and the character of the distribution of the internal heat sources. We show that under the action of the heat sources a transition is possible from the generalized Stefan problem to the classical problem and vice versa. This corresponds to the case when the isothermal zone formed (generalized Stefan problem) remains localized (classical Stefan problem) during the interaction process and then it can once again expand into a region of finite size. We formulate the conditions for such a transition as well as the conditions determining the change in the regime of development of the boundary of the isothermal region of both weak and strong discontinuities of the heat flux.

The numerical solution of the one-dimensional Stefan problem is based on the difference method for solving the one-dimensional heat-conduction equation using an implicit scheme and the sweep method [9] as well as a regular algorithm which we propose for changing the arrangement of the grid nodes as the boundary of the phase-transition region moves. The grid nodes move only near the boundary; other grid nodes remain stationary. The numerical algorithm makes it possible to determine both the displacement of the boundary itself and the change in temperature as a function of time in the corresponding regions. Other numerical algorithms are considered in [8, 10].

1. Formulation of the Problem. A plate of thickness H (the x axis is oriented perpendicular to the surface of the plate and is directed into the material) heated by distributed volume heat sources with density $q_V(x, t)$, $0 \le t \le T$, where T is the time during which the heat sources act, is studied in the coordinate system OYX. We designate the region $0 \le x \le H$ by $\Omega_0 = \{0, H\}$. The appearance of a phase-transition region depends on the phase-transformation temperature T_F and the heat energy of the phase transformation Q_F per unit mass of the material (in the case of melting, the appearance of the phase transition region depends on the specific heat of melting). We assume that the thermal characteristics of the material before and after the phase transformation are known and, for simplicity, that they are uniform

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in space and time. The initial temperature is T(x, 0) = 0. In the general case there can arise in the plate regions with temperature $T(x, t) > T_F$ (the region after the phase transformation Ω_F), $T(x, t) < T_F$ (the region before the phase transformation Ω), and $T = T_F$ (isothermal region, in which a phase transformation occurs, Ω_T). We note that the region Ω_T can be localized, as in the classical Stefan problem [8] (i.e., region of measure zero), or it can be extended, as in the generalized Stefan problem [7] (regions of measure greater than zero). Writing the one-dimensional heat-conduction equation in each of the characteristic regions, we have

$$\frac{\partial T}{\partial t} = R_1 \frac{\partial^2 T}{\partial x^2} + Q_1(x, t), \quad T < T_F, \ x \in \Omega,$$

$$\frac{\partial T}{\partial t} = R_2 \frac{\partial^2 T}{\partial x^2} + Q_2(x, t), \quad T > T_F, \ x \in \Omega_F; \tag{1.1}$$

$$T = T_F, \qquad x \in \Omega_T, \tag{1.2}$$

where $R_2 = \lambda_F/a_F$; $a_F = \rho_F c_F$; $R_1 = \lambda/a$; $a = \rho c$; $Q_1 = q_v/a$; $Q_2 = q_v/a_F$; λ_F, ρ_F, and c_F are the thermal conductivity, the density, and the heat capacity in the material after the phase transition; and, λ, ρ, and c are the same quantities before the phase transition. The region Ω_T also includes the boundary between Ω and Ω_F, if such a region exists, and for this reason Eq. (1.2) can be regarded as the boundary condition for Eq. (1.1) in this case.

Besides the condition (1.2), it is also necessary to write down an additional condition determining the evolution of the boundary of the phase transition. In what follows, we make such an analysis of the evolution of the region Ω_T as a function of the thermal regime. The standard flux or temperature boundary conditions can be imposed on the exterior surfaces of the plate.

2. Analysis of Possible Regimes of Evolution of the Boundaries of the Region of Phase Transformation. The classical and generalized Stefan problems are studied in, respectively, [7, 8]. It is well known [8] that in Stefan's problem the condition must be satisfied at the phase transition boundary $x_F(t)$

$$\frac{dx_F}{dt} = \frac{q^- - q^+}{Q_F \rho}. \tag{2.1}$$

Here $q^+ = -\lim\limits_{x\to x_F+0} \lambda \frac{\partial T}{\partial x}(x, t)$; $q^- = -\lim\limits_{x\to x_F-0} \lambda_F \frac{\partial T}{\partial x}(x, t)$; Q_F is the phase-transformation energy; and, ρ is the density of the material. It is assumed that $T \geq T_F$, $x \leq x_F$; $T \leq T_F$, $x \geq x_F$. At the boundary of the phase-transformation region the energy flux q has a discontinuity of the first kind.

A characteristic feature of the generalized Stefan problem is the presence of an extended isothermal zone (for example, with the boundary $\{x_F^{(1)}(t),\ x_F^{(2)}(t);\ x_F^{(1)} \leqslant x \leqslant x_F^{(2)},\ T = T_F\}$). A necessary condition for the formation of an extended isothermal zone is the presence of volume sources, which are presented in [7], where different boundary conditions on the boundary of this zone are established (aside from the condition $T = T_F$) and the question of the existence and uniqueness of the solution is considered. Thus, in the case when this zone expands $(\dot{x}_F^{(1)} \leqslant 0, \dot{x}_F^{(2)} \geqslant 0)$ the condition

$$\frac{\partial T}{\partial x} = 0, \tag{2.2}$$

must be satisfied. This condition corresponds to no heat flow out of the isothermal region as the region expands. We introduce the heat quantity $Q_S(x, t)$ $(x \in [x_F^{(1)}, x_F^{(2)}])$ absorbed per unit volume in the process of the phase transformation $Q_S \leq Q_F\rho$. When the absorbed heat energy Q_S reaches at some point of the region Ω_T the value ρQ_F the phase transformation process stops at this point. The energy required for the phase transformation in the isothermal zone is $\rho Q_F - Q_S$.

We now consider the case when the heat flux at the boundary of the isothermal region is different from zero. Assume first that the isothermal region adjoins the region before the phase transition, i.e., $x \geq x_F^{(2)}$, $T \leq T_F$. Then the flux $q^+ > 0$. Consider the heat-balance equation for a quite small region $\delta x_F^{(2)} < 0$ adjoining the boundary. The energy flowing out of this region is $q^+\delta t$, and the heat flowing into the region is $q_v \delta t \delta x_F^{(2)}$, which is a quantity of second order (in the limit $\delta x_F^{(2)} \to 0$) compared with $q^+\delta t$. Therefore, the thermal energy will start to decrease and crystallization will be the only possible process here. Then, in the leading-order approximation for the crystallization process $q^+\delta t = -(\rho Q_F + Q_s(x, t))\,\delta x_F^{(2)}$ we have the limit $\delta t \to 0, \delta x_F^{(2)} \to 0$

$$\frac{dx_F^{(2)}}{dt} = -\frac{q^+}{\rho Q_F + Q_s\left(x_F^{(2)}, t\right)}, \quad \dot{x}_F^{(2)} \leqslant 0. \tag{2.3}$$

Similarly, for $x_F^{(1)}$ in this regime $(\dot{x}_F^{(1)} \geqslant 0)$

$$\frac{dx_F^{(1)}}{dt} = \frac{q^-}{\rho Q_F + Q_s\left(x_F^{(1)}, t\right)}, \quad \dot{x}_F^{(1)} \geqslant 0. \tag{2.4}$$

If the isothermal region (for example, $x \geq x_F^{(1)}$, $T = T_F$)) adjoins the region of the material after the phase transition [$T(x_V, t) \geq T_F$, $x \leq x_F^{(1)}$], we have in the presence of a flux q^- into this region [7]

$$\frac{dx_F^{(1)}}{dt} = \frac{q^-}{\rho Q_F - Q_s\left(x_F^{(1)}, t\right)}. \tag{2.5}$$

The equations (2.1)-(2.5) describe the evolution of the phase-transformation zone or the isothermal zone. Besides these conditions, however, it is necessary to impose additional conditions which determine the thermal regime in which phase-trannformation regions develop according to one of the laws (2.1)-(2.5).

We now consider Stefan's problem. Let $x \leqslant x_F$, $T(x, t) \geqslant T_F$; $x \geqslant x_F$, $T \leqslant T_F$; $x_F > 0$, and let Eq. (2.1) hold on the boundary $x = x_F$. We now formulate the necessary and sufficient conditions for the appearance of an isothermal region at the time $t = t_0$. Formation of this region at $t \geq t_0$ means that there appears an isothermal region with the boundary $x_F^{(1)}(t)$, $x_F^{(2)}(t), x_F^{(2)}(t) > x_F^{(1)}(t), \dot{x}_F^{(2)}(t) > \dot{x}_F^{(1)}(t), t > t_0$ at $t = t_0, x_F^{(1)} = x_F^{(2)} = x_F(t_0)$.

A necessary condition at the moment $t = t_0$ for the formation of an isothermal zone is $q^+(x_F, t_0) = 0$. Indeed, if an isothermal region could form at $t = t_0 + \delta t (\delta t \to 0)$ with $q^+ > 0$, then on its boundary $q^+\left(x_F^{(2)}, t_0 + \delta t\right) > 0\ (\delta t \to 0)$ and, according to the proof given above, the crystallization process would begin and $\dot{x}_F^{(2)} < 0$, which is impossible, since by convention $\dot{x}_F^{(2)} > 0$. Therefore, if the isothermal region forms at $t = t_0$, there is no heat flux $q^+ = 0$.

A sufficient condition for the formation of an isothermal zone is thet the temperature increase $T \geq T_F$ for $x \gtrsim x_F(t_0 + \delta t)$ and $\delta t \gtrsim 0$ $(\delta t \to 0)$, i.e., near the boundary x_F, under the necessary condition $q^+ = 0$. Indeed, if this is the case, then at $t = t_0 + \delta t$ a zone where $T > T_F$ forms in front of the boundary of the phase-transformation region x_F; this is impossible within Stefan's classical problem and means that a phase transition must start at these points, i.e., an isothermal zone forms and a transition to the generalized Stefan problem occurs.

We now consider the question of the possible change in the evolution regime of the isothermal region from expansion ($\dot{x}_F^{(2)} > 0$) (2.2) to contraction ($\dot{x}_F^{(2)} < 0$) (2.3). Let at $t = t_0$ the boundary of the isothermal zone be $x_F^{(2)}$, on which the solution satisfies the condition (2.2). In order that the isothermal region continue expanding at $t > t_0$, i.e., $\delta x_F^{(2)} > 0$, it is necessary that at $t = t_0 + \delta t$, under the boundary condition (1.2), and at the fixed boundary $x_F^{(2)}$ the flux $q^+\left(x_F^{(2)}, t_0 + \delta t\right) < 0$ (i.e., for $x \gtrsim x_F^{(2)}(t_0)$ the temperature increases: $T(x, t_0 + \delta t) \gtrsim T_F$). Indeed, if this is not the case, then $q^+ > 0$ and hence the crystallization process arises from the boundary $x_F^{(2)}$ and the isothermal region does not form. These assertions must be checked at each step in time. This will make it possible to follow the change in the regime of development of the phase-transformation region.

The possible change in the regime of development of the phase-transition region from Stefan's condition (when the phase-transition region is localized) to the generalized Stefan problem (appearance of an extended isothermal phase-transformation region) and vice versa is illustrated below in numerical examples. In order to find the temperature distribution in the presence of characteristic regions, whose development will be determined by one of the conditions (2.1)-(2.5), it is necessary to give a regular procedure for finding the solution of Eq. (1.1) in these regions.

3. Numerical Algorithm for Determining the Motion of the Boundaries of the Phase Transition and Constructing the Solution of the Heat-Condition Equation. According to the analysis performed above, a plate of thickness H at the start of the phase-transformation process separates into characteristic regions on whose boundaries the condition (1.2) is satisfied. We now study an algorithm for constructing a numerical solution in this case. Since the boundary on which the condition (1.2) holds moves, the nodes partitioning the region will also move. In [10] two coordinate systems were introduced in order to find the solution in the characteristic regions: mobile and stationary; the mobile coordinate system was chosen in the entire region where the solution was sought.

In the method proposed below the mobile coordinate system is used only in the neighborhood of the motion of an unknown boundary; all other grid nodes are stationary. In this way we quantize the region whose boundary moves according to the conditions (2.1) and (2.3)-(2.5).

Let x_F be the phase-transformation boundary, whose motion is determined by one of the conditions (2.1) and (2.3)-(2.5). We first take Stefan's condition, when the solution of the heat-conduction equation must be sought for $x > x_F (T < T_F)$ and $x < x_F (T > T_F)$. Let $x_j (j = 1, \ldots, N)$ be the nodes of the grid partitioning the plate, and let $\Delta_j = x_{j+1} - x_j$ $(j = 1, \ldots, N - 1)$ be the grid step. We assume that $x_F = x_j$ at $t = t_0$. Then we proceed as follows. We displace the point x_{j+1} into x_j and we obtain in the region $x_F \leq x \leq H$ a new partition with nodes $\xi_{j+1}, x_{j+2}, \ldots, x_N$. Here ξ_{j+1} is a new node, and the grid step $\Delta'_{j+1}, \Delta_{j+2}, \ldots, \Delta_{N-1}$, $\Delta'_{j+1} = x_{j+2} - x_F$ (at the first step $x_F = x_j$). The region $0 \leq x \leq x_F$, however, is partitioned by the nodes $x_1, \ldots, x_{j-1}, \xi_j$ $(\xi_j = x_j)$, at the first step $t = t_0$, and the grid step $\Delta_1, \ldots, \Delta'_{j-1}$, where $\Delta'_{j-1} = x_F - x_{j-1}$ $(x_F = x_j$ at $t = t_0)$. The boundary $\xi_j = \xi_{j+1}$ for these regions will move in accordance with the condition (2.1), the fluxes and temperatures in which are calculated at the preceding step

$$\delta\xi_j = \delta\xi_{j+1} = -(q^- - q^+)\delta t/\rho Q_F \equiv \delta x_F \tag{3.1}$$

where δt is the time step. The temperature at the point ξ_{j+1} at the preceding time step is calculated according to the linear approximation

$$T_{j+1}(t) = T_F + [(T_{j+2} - T_F)\,\delta\xi_{j+1}/\Delta'_{j+1} = T_j(t).$$

Thus, the nodes $\xi_j = \xi_{j+1}$ move continuously with time. As soon as the node ξ_j reaches x_{j+1} (i.e., $\xi_{j+1} = x_{j+1}$), we return to the old nodes x_j and x_{j+1}. At x_{j+1} the temperature $T_{j+1} = T_F$, and at x_j, we approximate the temperature by the linear law $T_j = T_F - (T_F - T_{j-1}) \times (x_{j+1} - x_j)/\Delta'_{j-1}$. After this, we displace x_{j+2} into x_{j+1} and repeat the entire procedure. As a result we obtain an algorithm for changing the grid as the nodes move. At each moment in time the heat-conduction equations (1.1) were solved numerically by an implicit scheme using the sweep method [9] along the nodes chosen in the manner described above.

If the region of the phase transformation $(T > T_F)$ adjoins the isothermal region (for example, we take the boundary $x_F = x_F^{(1)}$), then the motion of the boundary is found for one of the conditions (2.4) or (2.5). Then in each region the grid is chosen according to the algorithm described above, and the displacement of the nodes will be determined, correspondingly, by $\delta\xi_j = \delta\xi_{j+1} = \delta t q^-/(\rho Q_F \pm Q_s) > 0$ (sign (+ or −) depends on the character of the phase-transformation process). A similar condition is written for the boundary $x_F^{(2)}(t)$. When the isothermal zone is localized, its motion is described by the relation (3.1).

We now consider the case of expansion of the isothermal zone according to the condition (1.2) and (2.2), choosing the static grid $x_1, \ldots, x_N$ in the entire strip.

Let $x_j = x_F$ be the boundary of the isothermal region $(T = T_F,\ x < x_F)$. Then the heat-condition equation (1.1) is solved numerically along the grid with the nodes $x_j, \ldots, x_N$ under the boundary condition (2.2). Displacement of this region into the next node was determined from the condition that the temperature at the boundary x_j reached the prescribed value $T_j = T_F - \varepsilon$, where ε determines how closely T_F is approached.

Thus, we have proposed a numerical algorithm for finding the temperature distributions in different characteristic regions. We consider below different examples of the appearance and development of phase-transition regions, taking into account the isothermal zone and its localization and possible reappearance. We note that the proposed algorithm for describing the evolution of each of the three regions $(\Omega, \Omega_T, \Omega_F)$ can be used for any number and combination of the indicated regions, and the solution inside the regions themselves will be found

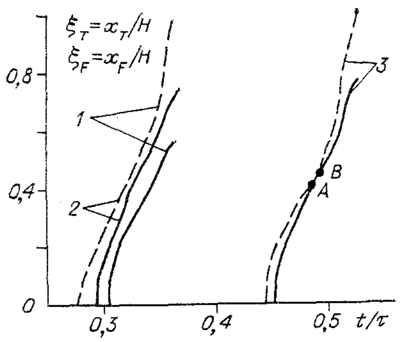

Fig. 1

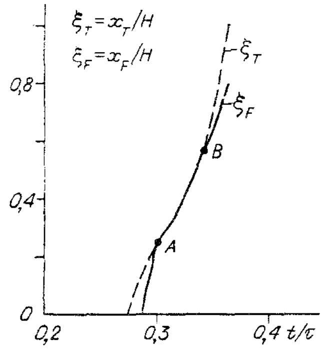

Fig. 2

with the help of an implicit scheme by the sweep method. The assertions proved above and the proposed computational algorithm also remain valid for nonuniform thermophysical parameters.

4. Numerical Examples. We considered a strip of thickness H and a distribution of volume sources $q_V = Ae^{-\alpha\xi}$, where $\xi = x/H$ and A and α are parameters. The surfaces of the strip are thermally insulated, and the initial temperature is $T(0, x) = 0$ (if $T(0, x) = T_0 = \text{const}$, then the calculations presented below correspond to $\Delta T = T - T_0$). Before starting the computational process, it is convenient to make the physical quantities dimensionless: the time $t' = t/\tau$ and the coordinate $\xi = x/H$, where $\tau = aH^2/\lambda$. Then in Eq. (1.1) we have $R_1 = 1$, $Q_1 = q_v H^2/\lambda$, $Q_2 = q_v H^2 a/\lambda a_F \equiv Q_1 a/a_F$, $R_2 = \lambda_F a/a_F\lambda$, $A' = AH^2/\lambda$ [use t' instead of t and ξ instead of x in Eq. (1.1)]. We also introduce the quantities $Q_F' = \rho Q_F/a$, $Q_s' = Q_s/a$ and the fluxes $q^+ = -\partial T/\partial\xi (T < T_F)$, $q^- = -\lambda_F\lambda^{-1}\partial T/\partial\xi$ for $T > T_F$ (Q'_F, Q'_S, q^+, q^- in degrees). Then the conditions (2.1) and (2.3)-(2.5) can be written in the dimensionless form ($\xi = x_F/H$ or $\xi = x_F^{(1)}/H$)

$$\frac{d\xi}{dt'} = \frac{q^- - q^+}{Q_F' \pm Q_s'} \quad \left(q^+ = 0 \text{ at } \xi = \frac{x_F^{(1)}}{H}\right). \tag{4.1}$$

The equations (1.1), written in the dimensionless form in the variables (ξ, t') with the condition (4.1), were implemented numerically by the method described above. As a result, the motion of the boundaries of the characteristic regions was calculated as a function of the time t'.

Figure 1 displays a number of curves of the development of the boundaries of the characteristic regions as a function of the parameters R_2, Q'_F, T_F, and A'. The isothermal region formed from the boundary $\xi = 0$ and is designated by the dashed line $(\xi_T = x_F^{(2)}(t)/H)$, while the phase-transition region $(\xi_F = x_F^{(1)}(t)/H)$ is denoted by the solid line. The calculations were performed for the parameters $T_F = 1$, $a = a_F$, $R_2 = 1$, $A' = 5$, $\alpha = 1$, and $Q'_F = 0.1$; 0.05 (curves 1 and 2). The motion of the boundary of the isothermal zone did not change, since the the boundary of the phase-transition zone did not "overtake" the boundary of the isothermal zone. The motion of the phase boundary, however, "accelerated." This is connected with the decrease in the phase-transformation energy.

The development of the phase-transition region for the same parameters as above and $Q'_F = 0.03$ is shown in Fig. 2. The boundary of the phase-transformation region "overtakes" the boundary of the isothermal region (point A, Fig. 2), and this region becomes localized, i.e., the generalized Stefan problem transforms into the classical Stefan problem. In the process, the velocity of the phase-transformation boundary decreases, since $Q'_S(\xi, t') = 0$. The phase-transition boundary then propagates in accordance with the condition (2.1) (the section AB, Fig. 2). The slow down of the boundary of the phase-transformation region results in heating of the material in the region before the phase transformation from the volume sources in it and the possibility of formation of an isothermal zone (point B, Fig. 2) in accordance with the criterion formulated above; it then propagates up to the boundary of the strip. Thus, the decrease in the absorption energy "accelerates" the boundary of the isothermal zone and the region of the material after the phase transformation and results in the seemingly "oscillatory" development of an isothermal zone — from finite size to localized and vice versa.

An increase in the phase-transition temperature leads to a similar effect. Figure 1 displays (curve 3) the time dependence of the position of the boundary for $A' = 5$, $\alpha = 1$,

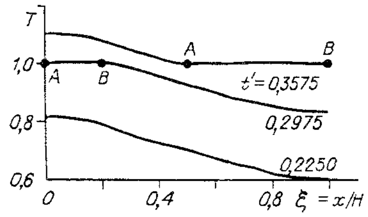

Fig. 3

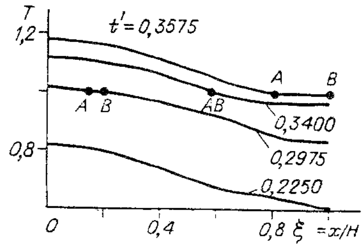

Fig. 4

Q'_F = 0.05 and T_F = 1.5. It is obvious that an increase in the phase-transition temperature slows down the motion of the isothermal region and makes it possible for this region to be localized.

Figures 3 and 4 display the temperature distribution over the thickness of the plate for different times t'. The temperature distribution in Fig. 3 corresponds to curve 1 in Fig. 1 and its thermal parameters and the distribution in Fig. 4 corresponds to the curve of Fig. 2 and its thermal parameters (the section AB in these figures is the isothermal zone). Figure 4 shows the formation, localization, and then expansion (the section AB) of the isothermal zone.

Thus, the method proposed above was used to perform calculations of the evolution of the motion of the boundaries of characteristic regions as a function of time. It was shown that the phase-transformation regime can change from a localized isothermal region to a finite region and vice versa. This must be taken into account in real problems, since it can substantially influence the property of the material in front of a phase-transformation region and it will also make possible the creation of extended isothermal regions and thereby influence the properties of the material with smaller energy expenditures than that required for a phase transition. This latter property makes volume heat sources (in particular, microwave radiation) promising for fracturing or weakening an entire series of materials.

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