APPROXIMATE SOLUTIONS OF THE HEAT CONDUCTION EQUATION IN THE ONE-DIMENSIONAL CASE WITH PHASE TRANSITIONS ON THE OUTER SURFACE OF A BODY

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Approximate solutions are presented for the heat conduction equation for a semi-infinite rod or half-space with sublimation at its outside boundary. The formulas presented are in a form convenient for practical computations.

Because of the intensive development of high-temperature research much attention has recently been given to the question of heat transfer accompanied by phase transitions on the boundary of a body. Because the problem is a complex one, solution of these problems is often attempted with the aid of electronic computers, for example, as in [1] and a number of other papers. However, in the majority of cases it is useful to have an approximate solution which can describe, however qualitatively, the phenomenon under examination.

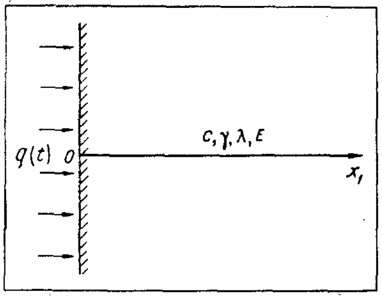

Fig. 1. Schematic illustration of the problem.

We assume that a homogeneous bar of material, subliming from the solid phase under certain conditions without transition through the liquid phase, is heated from one end (Fig. 1). After a certain initial interval, associated with the heating of the end of the bar, a time comes when the sublimation temperature T_S is reached on the boundary of the body. We shall take this instant as the beginning of the process to be studied.

This schematization of the problem of heat propagation is equivalent to an analogous problem for the heat conduction equation in the case of a half-space when the conditions on the boundary are independent of the location of the point considered. In the first case, on the assumption that the lateral surface of the bar is thermally insulated, and in the second case — as a result of the symmetry of the temperature field resulting from the symmetry of the heat fluxes at the body surface, the problem reduces to solution of the one-dimensional heat conduction equation

$$a\frac{\partial^2 T(x_1, t)}{\partial x_1^2} - \frac{\partial T(x_1, t)}{\partial t} = 0 \quad \text{for } \xi(t) \leqslant x_1 < \infty. \qquad (1)$$

The boundary conditions are

$$T(\xi, t) = T_s = \text{const}, \qquad (2)$$

$$q(t) + \lambda\frac{\partial T(x_1, t)}{\partial x_1} - E\gamma\dot{\xi} = 0 \quad \text{for } x_1 = \xi, \qquad (3)$$

$$T(x_1, t) \to T_0 = \text{const} \quad \text{for } x_1 \to \infty, \qquad (4)$$

$$\frac{\partial T(x_1, t)}{\partial x_1} \to 0 \quad \text{for } x_1 \to \infty. \qquad (5)$$

At time zero there is a certain temperature distribution and the sublimation front is at rest

$$T(x_1, 0) = f(x_1), \qquad (6)$$

$$\xi(0) = \dot{\xi}(0) = 0. \qquad (7)$$

In writing Eqs. (1) — (7) the assumption is made that the thermophysical properties of the material are constant.

This problem was examined in [2] under conditions of constancy of heat flux at the body surface. Attempts have also been made to solve the above problem with various simplifying assumptions regarding the nature of the dependence of heat flux on time q = q(t) or on the rate of propagation $\dot{\xi} = \dot{\xi}(t)$ of the sublimation front. A description follows of an approximate method of solution of Eq. (1) with boundary and initial conditions (2)–(7).

We shall go over to a new space coordinate, taking an origin coincident with the moving sublimation front,

$$x = x_1 - \xi. \qquad (8)$$

Then Eqs. (1)–(3) take the form

$$a\frac{\partial^2 T(x, t)}{\partial x^2} + \dot{\xi}\frac{\partial T(x, t)}{\partial x} - \frac{\partial T(x, t)}{\partial t} = 0 \quad \text{for } 0 \leqslant x < \infty, \qquad (9)$$

$$T(0, t) = T_s, \qquad (10)$$

$$q(t) + \lambda\frac{\partial T(x, t)}{\partial x} - \gamma E\dot{\xi} = 0 \quad \text{for } x = 0. \qquad (11)$$

In place of the conditions at infinity, as in [2], we shal make the assumption that the temperature of the material differs from its initial value only in a layer of a certain thickness δ(t) adjacent to the phase transition surface. We shall call it the heat-assimilation layer, since all the heat arriving at the body accumulates in this layer. Then Eqs. (4) and (5) are amended as follows:

$$T(\delta,\ t) = T_0, \tag{12}$$

$$\frac{\partial T(x,\ t)}{\partial x} = 0 \text{ for } x = \delta(t). \tag{13}$$

We also require that Eq. (9) be satisfied only on the average for the layer of thickness δ(t), for which purpose we integrate it with respect to x from x = 0 to x = = δ(t). Using the boundary conditions (10)–(13), we obtain

$$\frac{d}{dt}(\Theta - T_0\delta) = \frac{q(t)}{c\gamma} - \left(\frac{E}{c} + T_s - T_0\right)\dot{\xi}, \tag{14}$$

where $\Theta(t) = \int\limits_0^\delta T(x,\ t)\,dx$ and c is the specific heat of the material.

Equations (11) and (14) determine the unknown functions ξ(t) and δ(t). The dependence of Θ(t) and T(x, t) must be found from additional considerations. We note that Eq. (14) integrates in the final form,

$$\xi(t) = \int\limits_0^t \frac{q(t)}{\gamma I_{\text{eff}}}\,dt - \frac{c}{I_{\text{eff}}}\left[\Theta - \Theta_0 - (\delta - \delta_0)T_0\right], \tag{15}$$

where $I_{\text{eff}} = E + c(T_s - T_0)$ is the so-called effective enthalpy of the material and Θ_0, δ_0 are the initial values of the quantities indicated.

We shall make the approximation that the temperature profile T(x, t) in the layer 0 ≤ x ≤ δ(t) is close to the quadratic form

$$T(x,\ t) = A(t) + B(t)x + C(t)x^2.$$

By satisfying the boundary conditions (10), (12), and (13), we obtain the following expression for the dependence of T(x, t):

$$T(x,\ t) = T_0 + (T_s - T_0)\left[1 - x/\delta(t)\right]^2. \tag{16}$$

Substituting (16) into Eq. (11), we have

$$q(t) - 2\lambda(T_s - T_0)/\delta(t) = \gamma E\dot{\xi}. \tag{17}$$

On the other hand, evaluating the quantity Θ(t), taking account of (16), and substituting the result obtained into (15), we obtain a second equation to determine ξ(t) and δ(t),

$$\xi(t) = \int\limits_0^t \frac{q(t)}{\gamma I_{\text{eff}}}\,dt - \frac{c}{3I_{\text{eff}}}(T_s - T_0)(\delta - \delta_0). \tag{18}$$

Thus, we have obtained a first integral of the system of differential equations (9), (14). For a complete solution of this system we need a second integral. With this objective we eliminate from Eqs. (17) and (18) the quantity ξ(t), to achieve which we differentiate (18) with respect to t and substitute the expression obtained for $\dot{\xi}$ into (17). After elementary transformations we reduce the expression obtained to the following form:

$$\frac{d\delta(t)}{dt} = \frac{6aI_{\text{eff}}}{E\delta} - \frac{3}{\gamma E}\,q(t). \tag{19}$$

Solutions of the differential equation (19) with the initial condition δ(0) = δ_0 gives the above-mentioned second integral. We shall consider separately the cases of constant and variable heat flux at the body surface.

The case of constant heat flux, q = const. The solution described below differs from the analogous result of [2] as regards the method. Use of the moving coordinate (8) allows us to obtain the solution of the problem by a shorter method, while the result is expressed in a simple form suitable for analysis and practical computation. Moreover, thanks to the solution that has been obtained, it is possible to construct an approximate solution for the case q(t) ≠ const. In the case q = const Eq. (19) is easily integrated, and we obtain the following expression for the thickness of the heat-assimilation layer:

$$\delta(t) = \delta_0 - \frac{3q}{\gamma E}\,t - \frac{2\lambda I_{\text{eff}}}{cq}\ln\left[1 - \frac{\delta/\delta_0 - 1}{2\lambda I_{\text{eff}}/cq\,\delta_0 - 1}\right]. \tag{20}$$

We shall now consider what the quantity δ_0 is. According to the definition it is the thickness of the heat-assimilation layer at the time when the temperature at the outer boundary reaches the value T_s. It is easy to see [2] that up to the start of sublimation, the temperature in the heat-assimilation layer, when given in the form of a quadratic expression, is determined according to the law

$$T(x,\ t) = T_0 + \frac{q\delta(t)}{2\lambda}\left(1 - \frac{x}{\delta}\right)^2.$$

Hence for δ_0 a simple formula is obtained,

$$\delta_0 = 2\lambda(T_s - T_0)/q. \tag{21}$$

Substituting (21) into (20), and introducing the notation

$$k = I_{\text{eff}}/c(T_s - T_0) - 1, \tag{22}$$

we reduce (20) to the following form:

$$\delta(t) = \delta_0 - \frac{3qt}{\gamma E} - \frac{2\lambda I_{\text{eff}}}{cq}\ln\left[1 - \frac{\delta/\delta_0 - 1}{k}\right]. \tag{23}$$

Thus, Eqs. (18) and (23) determine the magnitude of the entrained layer and the thickness of the heat-assimilation layer as a function of time.

For convenience of theoretical analysis and practical calculation we introduce the parameter m as follows:

$$\delta(t) = (1 + km)\delta_0. \tag{24}$$

Substituting (22) and (24) into (23), and carrying out simple transformations, we write the latter in the dimensionless form

$$\frac{t}{p} = -\frac{k}{k+1}\left[\frac{k}{k+1}\,m + \ln(1 - m)\right], \tag{25}$$

where $p = 2\lambda\gamma I_{\text{eff}}^2/3cq^2$ is a quantity having the dimension of time. It may be seen from expression (25) that m =

$= 0$ corresponds to time $t = 0$, while $m \to 1$ corresponds to $t \to \infty$, i.e., the range of variation of the parameter m: $0 \le m < 1$ corresponds to the infinite time interval $0 \le t < \infty$. It is seen immediately that when the parameter m is varied in the above range, the right side of (25) increases monotonically, starting at zero. Therefore, relation (25) establishes a single-valued correspondence between the true time t and the artificial parameter m.

Substituting (22) and (24) into Eq. (18), we express the subliming layer of material in the following form:

$$\xi(t) = \int_0^t \frac{q}{\gamma l_{\mathrm{eff}}}\,dt - \frac{1}{3}\,\frac{k}{k+1}\,\delta_0 m. \qquad (26)$$

Formula (26) is a semiparametric expression for the dependence $\eta = \xi(t)$, where the parameter is the quantity m, connected with the time t by relation (25). Using the above relation, it is easy to establish the degree of approximation of the values of the quantity $\xi(t)$ to the asymptotic relation given by the expression

$$\xi(t) = \int_0^t \frac{q\,dt}{\gamma l_{\mathrm{eff}}} - \frac{1}{3}\,\frac{k}{k+1}\,\delta_0. \qquad (27)$$

It is seen from (25) that as t increases the parameter m tends very quickly to unity. In cases of practical importance the quantity m is close to unity, apart from a short initial time interval, in which formula (27) may be used. This noteworthy feature is a consequence of the fact that in the chosen moving coordinate system the thickness of the heat-assimilation layer $\delta(t)$ tends to a constant value $\delta_{\max}$ as $t \to \infty$. It follows from (24) that

$$\delta_{\max} = (1 + k)\,\delta_0. \qquad (28)$$

It is of interest to evaluate the sublimation rate $\mathring{\xi}(t)$. Taking the derivative of (26) and using (25), we find

$$\dot{\xi}(t) = \frac{q}{\gamma l_{\mathrm{eff}}} - \frac{1}{3}\,\frac{\delta_0}{p}\,\frac{k+1}{1+km}\,(1 - m). \qquad (29)$$

Hence it is clear that during the above-mentioned time interval, the rate of sublimation is close to the constant value $q/\gamma l_{\mathrm{eff}}$. By replacing the quantities δ_0, k, p in (29) by the original thermophysical properties, it is not difficult to establish that $\xi(0) = 0$ (and then $m = 0$). This corresponds to the initial conditions of the problem.

Thus, by using formulas (26) and (29), and calculating the parameter m from relations (25), we may determine the value of the layer that has been removed and the rate of sublimation of the material of a semi-infinite bar of a half-space at any instant time. Calculation of the quantity $\xi(t)$ may be simplified by approximating to the dependence $\delta(t)$ by the exponential function

$$\delta(t) = \delta_0\,[1 + k\,(1 - \exp(-\alpha t))]. \qquad (30)$$

It is clear that the boundary conditions $\delta(0) = 0$ and $\delta(\infty) = \delta_{\max}$ are satisfied. The exponent α must be chosen so that the results of calculations according to (30) best coincide with the corresponding values obtained with the aid of (24) in the initial section, where the quantity m differs noticeably from unity. As calculation has shown, satisfactory agreement is obtained if α is determined from the condition that the two expressions for $\delta(t)$ coincide at the time when the difference $\delta - \delta_0$ attains 3/4 of its maximum value. Then we obtain the following relation for α:

$$\alpha = 2.77 \sqrt{p\,\frac{k}{k+1}\left(1.85 - \frac{k}{k+1}\right)}. \qquad (31)$$

For convenience of calculation we write (26) in the dimensionless form

$$\bar{\xi}(\bar{t}) = \frac{(k+1)\,\tau\bar{t}}{3} - \frac{1}{3}\,\frac{k}{k+1}\,m, \qquad (32)$$

where $\bar{\xi}(\bar{t}) = \xi(t)/\delta_0$; $\bar{t} = t/t_{\max}$; $\tau = t_{\max}/p$; and $t_{\max}$ is the total time of the sublimation process.

The analogous expression when the approximation (30) is used takes the form

$$\bar{\xi}(\bar{t}) = \frac{k+1}{3}\,\tau\bar{t} - \frac{1}{3}\,\frac{k}{k+1}\,[1 - \exp(-\alpha p \tau \bar{t})]. \qquad (33)$$

Figure 2 shows the results of calculation of the quantity $\bar{\xi}(\bar{t})$ according to formulas (25) and (32), compared with the results of solving the original system (1)–(7) by a numerical method on a computer. For comparison the same figure gives the results of calculation of the quantity $\bar{\xi}(\bar{t})$ with the aid of a simplified formula obtained from (32) or (26) by dropping the second term on the right side. In practice, calculation of the quantity $\bar{\xi}(\bar{t})$ from the approximate relation (33) gives the same results as calculation from (32). On the graph the curves corresponding to the above relations run together. Comparison of the curves shows good agreement with the results of calculations obtained by other methods.

The case of variable heat flux $q = q(t)$. We shall represent the heat flux in the form of a sum

$$q(t) = q_0 + q_1(t), \qquad (34)$$

where q_0 = const is the heat flux at the initial time $t = 0$ when the sublimation temperature is first obtained on the outside surface; $q_1(t)$ is the quantity determined by assigning the dependence $q(t)$; evidently $q_1(0) = 0$.

Returning to the solution of Eqs. (18) and (19), we note that the integral (18) remains unchanged. Thus, the matter reduces to solution of Eq. (19) with a free term depending on time. It is not possible to integrate this equation in exact form, and we therefore apply the following approximate method. We write Eq. (19), taking account of (34), as

$$\frac{d\delta}{dt} = \frac{6 a l_{\mathrm{eff}}}{E\delta} - \frac{3}{\gamma E}\,q_0 - \frac{3}{\gamma E}\,q_1(t). \qquad (35)$$

We seek a solution of Eq. (35) in the form of a sum

$$\delta(t) = \delta_1(t) + f(t), \qquad (36)$$

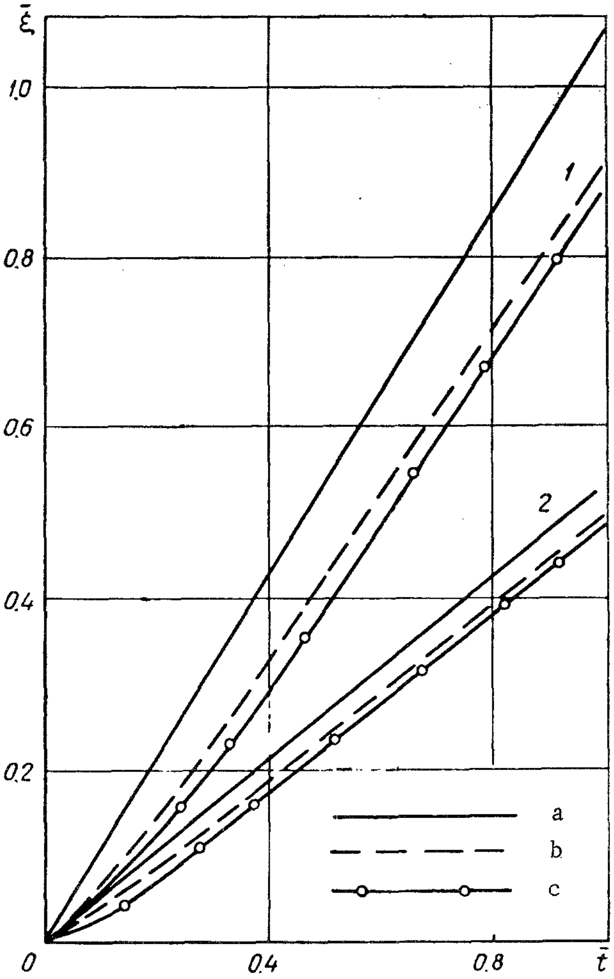

Fig. 2. Dependence of the sublimation of the material $\bar{\xi}$ on the conditions at the body surface and on the time $\bar{t}$: 1) for $k = 1.5$, $\tau = 1.256$; 2) $k = 0.33$, $\tau = 2.32$; a) according to the equation $\bar{\xi}(t) = (k + 1)\tau\bar{t}/3)$; b) numerical solution on a computer; c) calculation according to formulas (25) and (32).

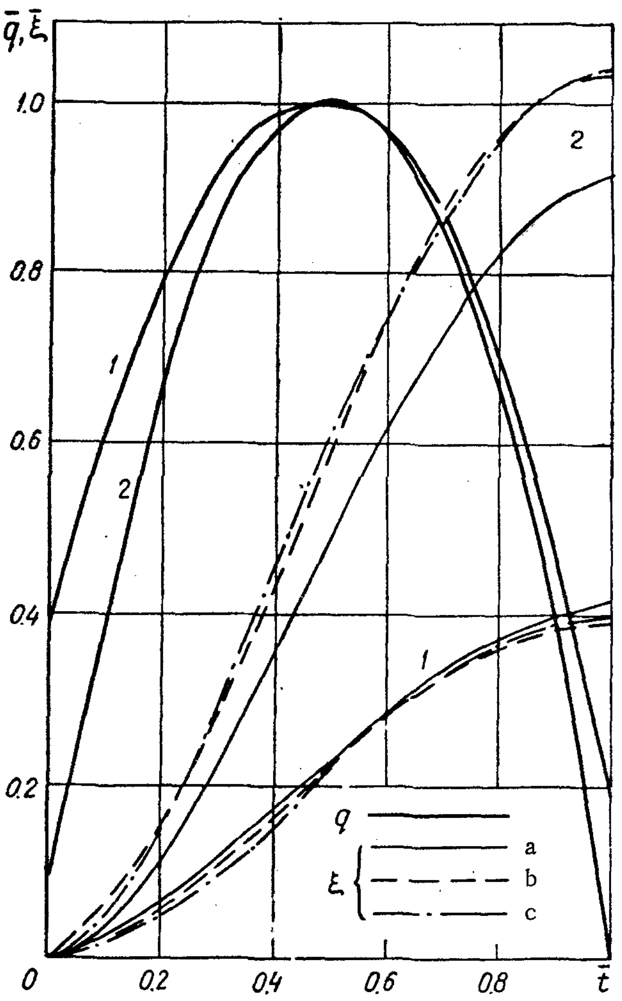

Fig. 3. Sublimation $\bar{\xi}$ of the material as a function of time for a variable heat flux at the boundary $k = 1.756$, $\tau = 0.224$ (1) and 0.113 (2): a) from the equation b) numerical solution on a computer; c) calculation from formulas (45), (46).

where $\delta_1(t)$ is a solution of the equation

$$\frac{d\delta}{dt} = \frac{6al_{\text{eff}}}{E\delta} - \frac{3}{\gamma E}\, q_0; \tag{37}$$

and $f(t)$ is the deviation of $\delta(t)$ from the "stationary" (with $q = q_0 = \text{const}$) solution $\delta = \delta_1(t)$. As regards $f(t)$, we assume that it is small in comparison with $\delta_1(t)$, i.e.,

$$|f(t)| \ll \delta_1(t). \tag{38}$$

Substituting (36) into (35) we obtain

$$\frac{d\delta_1}{dt} + \frac{df}{dt} = \frac{6al_{\text{eff}}}{E(\delta_1 + f)} - \frac{3}{\gamma E}\, q_0 - \frac{3}{\gamma E}\, q_1(t). \tag{39}$$

Using the inequality (38), we write the first term on the right side of (39) in the form of a geometrical progression with common ratio f/δ_1. Considering the ratio f/δ_1 to be small enough, we leave only those terms of the series which contain f/δ_1 to a power not exceeding the first. Then Eq. (39) transforms to the approximate form

$$\frac{d\delta_1}{dt} - \frac{6al_{\text{eff}}}{E\delta_1} + \frac{3}{\gamma E}\, q_0 + \frac{df}{dt} = -\frac{6al_{\text{eff}}}{E\delta_1^2}\, f(t) - \frac{3}{\gamma E}\, q_1(t)$$

or, because of (37),

$$\frac{df}{dt} + \frac{6al_{\text{eff}}}{E\delta_1^2}\, f(t) = -\frac{3}{\gamma E}\, q_1(t). \tag{40}$$

Thus, to determine the function $f(t)$, we have obtained a linear differential equation of first order. Here we regard $\delta_1(t)$ to be a known function of time, since the solution of Eq. (37) with $q = q_0 = \text{const}$ has been obtained above.

According to the definition (36), we have the following initial condition for $f(t)$: $f(0) = 0$. The solution of (40) with the given initial condition is the function

$$f(t) = -\frac{3}{\gamma E} \exp\left(-6a\,\frac{k+1}{k} \int_0^t \frac{dt}{\delta_1^2(t)}\right) \times$$
$$\times \int_0^t q_1(t) \exp\left(6a\,\frac{k+1}{k} \int_0^t \frac{dt}{\delta_1^2(t)}\right). \tag{41}$$

Substituting (41) into (36), we obtain an expression for the dependence $\delta(t)$. Now the following relation is obtained for the thickness of the subliming layer, from (18), (22) and the expression obtained or $\delta(t)$:

$$\xi(t) = \int_0^t \frac{q(t)}{\gamma l_{\text{eff}}}\, dt -$$
$$-\frac{1}{3}\,\frac{1}{k+1}\Bigg[km\,\delta_0 - \frac{3}{\gamma E} \exp\left(-6a\,\frac{k+1}{k} \times\right.$$
$$\left.\times \int_0^t \frac{dt}{\delta_1^2(t)}\right) \int_0^t q_1(t) \exp\left(6a\,\frac{k+1}{k} \int_0^t \frac{dt}{\delta_1^2(t)}\right) dt\Bigg], \tag{42}$$

where, as before, the parameter m is related with the time t through (25) when $q = q_0$.

Thus, the approximate solution of the problem with variable heat flux $q = q(t)$ has been obtained in quadratures (42). The temperature profile is then determined by Eqs. (16), (36), and (41).

In cases when the function $f(t)$ is not small in comparison with $\delta_1(t)$, the solution obtained, generally speaking, will not be valid. Nevertheless, it may be applied even in these cases with specific limitations. Let us examine such a case. It is clear from expressions (36) and (41) that $f(t)$ should not exceed $\delta_1(t)$ in absolute magnitude for the same values of the arguments, since negative thicknesses of the heat-assimilation layer on $\delta(t)$ cannot exist physically. Therefore, we make the approximation $f(t) = -\delta_1(t)$ in cases when the left side of (41) becomes less than $-\delta_1(t)$. This will correspond to the regime of zero thickness of the heat-assimilation layer, $\delta(t) = 0$. Setting $\delta(t) = 0$ in Eq. (18) and taking account of (22), we may then write the formula for $\xi(t)$ in the following form:

$$\xi(t) = \int_0^t \frac{q(t)}{\gamma l_{\text{eff}}}\, dt + \frac{1}{3}\,\frac{1}{k+1}\,\delta_0, \tag{43}$$

where δ_0 is evaluated as before from (21) with $q = q_0$. As is seen from (43), calculation of the thickness of the subliming layer is simplified in this case. The physical meaning of (43) is that for specific conditions a heat transfer regime may be attained such that all the heat arriving is expended in subliming the material. This, however, corresponds to a stepwise form of temperature variation: $T(0, t) = T_s$ and $T(\Delta x, t) = T_0$, where Δx is a positive value which may be as small as we please. It is understood that this kind of explanation of the process of sublimation and heating of the bar is an approximation. The corresponding error may be evaluated by taking account of the main terms relative to the quantity f/δ_1 in solving Eq. (39).

It may be seen directly from formula (18) that in the initial period of sublimation it is possible to make the approximation that

$$\xi(t) = \int_0^t \frac{q(t)}{\gamma l_{\text{eff}}}\, dt. \tag{44}$$

The value of the above initial period is determined by the intensity of the heat flux at the boundary and by the thermophysical properties of the material. As time increases, it is necessary to use relation (42). For specific conditions the magnitude of the subliming layer is determined approximately by (43). The presence of a second term on the right of (43) is due to the fact that in the initial period a certain amount of heat accumulates in the heat-assimilation layer, and then—for a large enough rate of propagation of the sublimation front—this heat goes over "returns" as it were, to the subliming layers.

As in the preceding case, we write relations (42) and (43) in dimensionless form,

$$\bar{\xi}(\bar{t}) = \frac{k+1}{3}\,\tau \int_0^{\bar{t}} \bar{q}(\bar{t})\, d\bar{t} - \frac{1}{3}\,\frac{k}{k+1}\Bigg[m -$$

$$-\tau \exp\left(-\frac{(k+1)^3}{k}\tau\int\limits_0^{\bar{t}}\frac{d\bar{t}}{(1+km)^2}\right)\int\limits_0^{\bar{t}}\bar{q}_1(\bar{t})\times$$

$$\times\exp\left(\frac{(k+1)^3}{k}\tau\int\limits_0^{\bar{t}}\frac{d\bar{t}}{(1+km)^2}\right)d\bar{t}\Bigg], \tag{45}$$

$$\bar{\xi}(\bar{t}) = \frac{k+1}{3}\tau\int\limits_0^{\bar{t}}\bar{q}(\bar{t})\,d\bar{t} + \frac{1}{3}\,\frac{1}{k+1}, \tag{46}$$

where $\bar{q}(\bar{t}) = q(t)/q_0$; $\bar{q}_1(\bar{t}) = q_1(t)/q_0$.

The results of calculations of the quantity $\bar{\xi}(\bar{t})$ from formulas (45) and (46) are given in Fig. 3 and compared with the results of a solution of the original equation by a numerical method on a computer.

For convenience of examination, the heat fluxes have been referred to the maximum heat fluxes in each case, i.e., $\delta(t) = 0$. Here the calculation in case 1 was carried out completely according to formula (45). In case 2 calculation of the quantity $\bar{q} = q/q_{\max}$, in conformity with the above-mentioned condition $\delta(t) = 0$, was carried out according to formula (46), starting from the time $\bar{t} = 0.545$, when the above equality is satisfied. In addition, Fig. 3 also gives results of calculation of the thickness of the subliming layer according to the approximate relation (44). From the data presented it is clear that the approximate solutions obtained for the heat conduction equation describe, with an accuracy sufficient for practical applications, the process of heating and sublimation of a semi-infinite bar or a half-space, with heat flux at the body boundary given as an arbitrary function of time. For a course estimate of the thickness of the subliming layer we may use formula (44), which is in the nature of a first approximation in calculations of sublimation of materials subject to intensive heating.

NOTATION

x_1 is the coordinate measured along the length from the end of the bar; t is the time; $T(x_1, t)$ is the current temperature at section x_1; a is the thermal diffusivity of material; $\xi(t)$ is the coordinate of sublimation front; q(t) is the heat flux to external body surface; λ is the thermal conductivity of material. E is the latent heat of sublimation (vaporization) of material; γ is the density of material; $\dot{\xi} = d\xi/dt$ is the rate of propagation of sublimation front.

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