The approach developed to the solution of heat conduction problem in a three-dimensional formulation is "exact" to a definite extent, the error is due just to the numerical realization. Results obtained on its basis can be test data for the foundation of the reliability of different approximate models applied in the computation of laminar orthotropic slabs under thermal action.

## NOTATION

$\lambda_j$ (j = 1, 2, 3) and heat conduction coefficients of an orthotropic body; $T(x_i, b^{(\ell)})$ are temperatures on the slab face surfaces; q is the heat flux; $\alpha^{(\ell)}$ is the heat elimination coefficient; $T_c^{(\ell)}$ is the environment function, and $\ell$ = 0, n.

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# MATHEMATICAL MODELING OF THE PROCESS OF PLANE POLYMER FILM FORMATION

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The approximate solution is considered of a nonlinear nostationary problem of heat conduction with conjugate boundary conditions.

A number of papers [1, 2] that take account most completely of the factors exerting substantial influence on the progress of a process is devoted to the mathematical modeling of polymer film and fiber formation. However, the assumptions made therein do not permit description of the film formation on cooling rollers with the accuracy needed for practical purposes. The problem is solved for boundary conditions of the third kind in all the papers mentioned, including in [1-3] for symmetric boundary conditions. This does not correspond to the actual technological process since cooling from the rollers is considerably more intense than from the air. Moreover, the assumption about boundary conditions of the third kind for the heat transmission through the roller wall does not permit taking account of the nonlinearity of the temperature profile therein during heating, which results in substantial errors in the initial cooling period. In this case conjugate heat transfer conditions assuming the interdependence of the film and roller wall temperature fields must be given on the film-roller boundary. The dependence of the thermophysical properties on the degree of crystallinity is not taken into account in [1] and on the temperature in [2, 3]. Utilization of finite-difference methods [1-3] can cause significant difficulties in the practice of engineering optimization computations.

The problem of heat transfer and nonisothermal crystallization of polymer films on a cooling roller system is solved in this paper by linearization and use of the Foureri, Galerkin-Kantorovich, and Kutta-Merson methods. A number of assumptions is made is the construction of the mathematical model of the process. A one-dimensional problem is considered since the roller diameter and film width exceed its thickness significantly. The initial temperature of the polymer melt is constant and homogeneous, and the initial roller wall temperature are constant and equal to the cooling fluid temperatures. The polymer thermophysical properties are described by using a two-phase model and depend linearly on
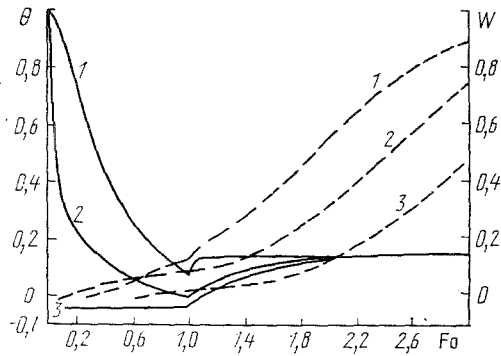
Fig. 1. Change in the temperature (solid lines) and the degree of crystallinity (dashes) during film cooling by two rollers; first roller Fo $\leq$ 1.0; second roller $1.0 \leq$ Fo $\leq$ 3.0; 1) $Y_1 = 0$; 2) 0.8; 3) 1.0.

both the temperature and on the degree of crystallinity, which is in good enough agreement with agreement theoretical and experimental data [4, 5]. A model that is a combination of the Avram equations, a model of autocatalytic type [6], and the kinetics equations of reactions of different order is proposed to describe the crystallization kinetics. The dependence of the crystallization rate on the temperature is described by an expression for a thermally activatable rate of nucleus formation in combination with a Williams—Lendell—Ferri expression for the activation energy [7]. Solution of an analogous problem for boundary conditions of the third kind [8] results from this as a particular case. Taking account of the assumptions elucidated above, the mathematical model of the heat transfer and non-isothermal crystallization of a polymer film on cooling rollers is written as follows:

$$\rho_1(T_1,\ W)\,C_1(T_1,\ W)\,\frac{\partial T_1}{\partial \tau} = \frac{\partial}{\partial y_1}\left[\lambda_1(T_1,\ W)\,\frac{\partial T_1}{\partial y_1}\right] + \tag{1}$$

$$+\ Q_{cr}\rho_1(T_1,\ W)\,\frac{\partial W}{\partial \tau},$$

$$\frac{\partial T_2}{\partial \tau} = a_2\,\frac{\partial^2 T_2}{\partial y^2}, \tag{2}$$

$$\lambda_1(T_1,\ W)\,\frac{\partial T_1(0,\ \tau)}{\partial y_1} - \alpha_1[T_1(0,\ \tau) - T_a] = 0, \tag{3}$$

$$T_1(h_1,\ \tau) = T_2(0,\ \tau), \tag{4}$$

$$\lambda_1(T_1,\ W)\,\frac{\partial T_1(h_1,\ \tau)}{\partial y_1} = \lambda_2\,\frac{\partial T_2(0,\ \tau)}{\partial y_2}, \tag{5}$$

$$\lambda_2\,\frac{\partial T_2(h_2,\ \tau)}{\partial y_2} + \alpha_2[T_2(h_2,\ \tau) - T_f] = 0, \tag{6}$$

$$T_1(y_1,\ +0) = T_1(h_1 - y_1,\ -0) = T_0(y_1), \tag{7}$$

for the first roller

$$T_1(y_1,\ 0) = T_0 = \text{const},\quad T_2(y_2,\ 0) = T_f = \text{const}, \tag{8}$$

$$\rho_1(T_1,\ W) = [\rho_L + \gamma_L(T_1 - T_L)](1 - W) + [\rho_c + \gamma_c(T_1 - T_c)]\,W, \tag{9}$$

$$c_1(T_1,\ W) = [c_L + \beta_L(T_1 - T_L)](1 - W) + [c_c + \beta_c(T_1 - T_c)]\,W, \tag{10}$$

$$\lambda_1(T_1,\ W) = [\lambda_L + \delta_L(T_1 - T_L)](1 - W) + [\lambda_c + \delta_c(T_1 - T_c)]\,W, \tag{11}$$

$$\frac{dW}{d\tau} = (1 - W)^m (r + sW)\,K(T_1)\,n\tau^{n-1}\exp\left[-\varepsilon\left(\frac{W}{1 - W}\right)^2\right], \tag{12}$$

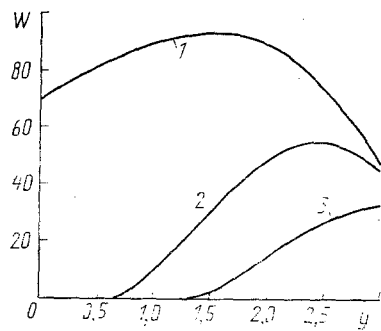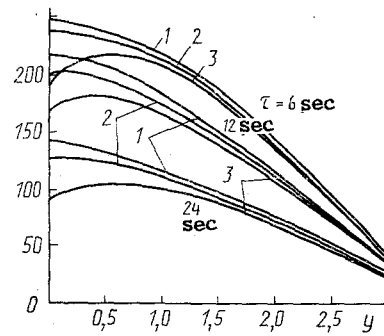$$K(T_1) = A\exp\left[-\frac{BT_1}{(T_1 - T_g + D)^2} - \frac{GT_m}{T_1(T_m - T_1)}\right]. \tag{13}$$

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Fig. 2. Distribution of the degree of crystallinity over the film section: 1) $\tau$ = 24 sec; 2) 12; 3) 6. W, %; y, mm.

Fig. 3. Transformation of the temperature profile over the film section: 1) $\alpha_1$ = 1 W/(m$^2$·K); 2) 15; 3) 70. T, °C.

According to the linearization method (Wideburg method), the system (1) and (2) with the boundary conditions (3)-(8) is solved initially for constant thermophysical properties and a zero heat of crystallization. The solution obtained by the Fourier method is the following in dimensionless form

$$\theta_1(Y_1,\ \text{Fo}) = u_1(Y_1) + \sum_{i=1}^{m} \xi_i \exp\left(-\mu_i^2\,\text{Fo}\right)\sin\left(\frac{\mu_i}{\sqrt{\tilde{a}_L}}Y_1 + \varphi_{1i}\right), \tag{14}$$

$$\theta_2(Y_2,\ \text{Fo}) = u_2(Y_2) + \sum_{i=1}^{m} M_i\xi_i \exp\left(-\mu_i^2\,\text{Fo}\right)\sin\left(\frac{\mu_i}{\sqrt{\tilde{a}_L}}Y_2 + \varphi_{2i}\right), \tag{15}$$

$u_1(Y_1)$ and $u_2(Y_2)$ are found from the inhomogeneous boundary conditions. The first approximation found in this manner for the temperature is substituted in the expression describing the thermophysial properties and kinetics of the crystallization. The linearized system of equations is solved by the Galerkin–Kantorovich method. The solution has the following form

$$\theta_1(Y_1,\ \text{Fo}) = U_1(Y_1,\ \text{Fo}) + \sum_{i=1}^{m} \Phi_i(\text{Fo})\sin\left(\frac{\mu_i}{\sqrt{\tilde{a}_L}}Y_1 + \varphi_{1i}\right), \tag{16}$$

$$\theta_2(Y_2,\ \text{Fo}) = U_2(Y_2,\ \text{Fo}) + \sum_{i=1}^{m} \Phi_i(\text{Fo})M_i\sin\left(\frac{\mu_i}{\sqrt{\tilde{a}_L}}Y_2 + \varphi_{2i}\right), \tag{17}$$

$U_1(Y_1,\ \text{Fo})$ and $U_2(Y_2,\ \text{Fo})$ satisfy just the boundary conditions. The time functions $\Phi_i(\text{Fo})$ are found from the solution of the ordinary differential equations obtained from the ortho-gonality conditions for the residuals of (1) and (2) written in dimensionless form to the coordinate functions

$$\frac{d\Phi_i}{d\,\text{Fo}} = -\mu_i^2\Phi_i(\text{Fo}) + \psi_i(\text{Fo}), \tag{18}$$

$$\Phi_i(0) = \Phi_{0i},\quad i = 1,\ 2,\ \dots,\ m. \tag{19}$$

Equations (18) with the initial conditions (19) are solved by the Kutta–Merson method.

Results of computing the heat transfer and nonisothermal crystallization of a polymer film on a two roller system are presented in Fig. 1. The following values of the physical and technological parameters are taken for execution of the computations: $h_1$ = 1.0 mm, $h_2$ = 10 mm, $T_0$ = 250°C, $T_f$ = 70°C for the first roller, $T_f$ = 90°C for the second roller, $T_a$ = 50°C, $\rho_L$ = 1000 kg/m$^3$, $\rho_c$ = 1100 kg/m$^3$, $\gamma_L$ = −0.1 kg/(m$^3$·K), $\gamma_c$ = −0.2 kg/(m$^3$·K), $C_L$ = 2580 J/(kg·K), $C_c$ = 2700 J/(kg·K), $\beta_L$ = 4 J/(kg·K$^2$), $\beta_c$ = 5 J/(kg·K$^2$), $\lambda_L = \lambda_c$ = 0.25 W/(m·K), $\delta_L = \delta_c$ = 0, $T_L = T_c$ = 20°C, m = 1, r = 1.0, s = 40, n = 1, $\varepsilon$ = 0, A = 6420, B = 4224, D = 333, G = 225.8, $T_m$ = 228°C, $T_g$ = 60°C, $Q_{cr}$ = 167 W/kg, $\rho_2$ = 7800 kg/m$^3$, $C_2$ = 500 J/(kg·k), $\lambda_2$ = 45 W/(m·K), $\alpha_1$ = 15 W/(m$^2$·K), $\alpha_2$ = 4000 W/(m$^2$·K).

As is seen from Fig. 2, the substantial inhomogeneity of the degree of crystallinity over the film thickness is the reason for the difference in the supermolecular structure of the polymer in the different layers and the reduction of the film strength.

The influence of the heat elimination coefficient on the polymer-air boundary on the heat transfer is shown in Fig. 3. It is seen from the computations that a change in $\alpha_1$ from 1 to 70 W/(m²·K) results in considerable deformation of the temperature profile. Therefore, a deduction can be made about the necessity to take account of the heat elimination in air despite the fact that it is two orders of magnitude less intense than the heat elimination on the roller-cooling fluid boundary.

Computations performed for all possible polymers for a different quantity of cooling rollers and different additional assumption (the dependence of the thermophysical properties on just the temperature or on just the degree of crystallinity, absence of heat of crystallization, heat insulation condition from air, etc.) permitted making the following deduction. The introduction of at least one simplified assumption results in substantial distortion of the temperature and crystallinity profiles. In particular, replacement of the conjugate heat transfer conditions in the boundary conditions of the third kind distorts the crystallization pattern on the first roller in the computation for rapidly crystallizing polymers. Such a replacement is possible on subsequent rollers where the temperature gradients are considerably smaller and also for slowly crystallizing polymers. For low cooling rates the Avram equation and the model of autocatalytic type yield practically identical results while for high rates it is preferable to use the equations of autocatlaytic type. To obtain a sufficiently uniform distribution of the degree of crystallinity over the film section during the cooling process it is necessary to apply no less than three-four rollers, where the time of polymer residency in the first roller should be as small as possible.

## NOTATION

$\tau$ is the time; $y_1$ is the transverse film coordinate; $y_2$ is the transverse roller wall coordinate; $h_1$ is the film thickness; $h_2$ is the roller wall thickness; $T_1$ is the film temperature; $T_2$ is the roller wall temperature; $T_a$ is the air temperature; $T_f$ is the cooling fluid temperature; $\alpha_1$ is the heat elimination coefficient on the polymer-air boundary; $\alpha_2$ is the heat elimination coefficient on the roller wall-cooling fluid boundary; W is the degree of crystallinity; $Q_{cr}$ is the specific heat of crystallization; A, B, s, D, r, G, are crystallization kinetics constants; n is the Avram index; $T_g$ is the polymer vitrification temperature; $T_m$ is the polymer equiilibrium melting point; $\rho_1(T_1, W)$ is polymer density; $c_1(T_1, W)$ is the polymer specific heat; $\lambda_1(T_1, W)$ is the polymer heat conduction; $\rho_L$, $c_L$, $\lambda_L$ are the themrmophysical properties of the crystalline polymer at the temperature $T_c$; $\rho_c$, c, $\lambda_c$; are the temperature coefficient of the thermophysical properties of the polymer melt; $\gamma_c$, $\beta_c$, $\delta_c$ are the temperature coefficients of the thermophysical properties of the crystalline polymer; $\lambda_2$ is the heat conduction of the roller material; $a_2$ is the thermal

$$ Fo = \frac{a_L \tau}{h_1^2} ; \quad Y_1 = \frac{y_1}{h_1} ; \quad Y_2 = \frac{y_2}{h_2} ; \quad \theta_1 = \frac{T_1 - T_a}{T_0 - T_a} ; \quad \theta_2 = \frac{T_2 - T_a}{T_0 - T_a} ; \quad \tilde{a}_L = 1; \quad \tilde{a}_2 = \frac{a_2}{a_L} = \frac{a_2 \rho_L \, C_L}{\lambda_L} . $$

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