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NUMERICAL MODELING OF THE FORMING OF FIBER BUNDLES FROM POLYMER MELTS

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A mathematical model for the process of forming of synthetic fibers moving as a bundle is formulated. Three main versions are considered: forming of exposed bundles, forming in shafts with blowing, and stretching of fibers by means of an ejector. Low and high-speed forming regimes are also considered within the framework of the Maxwell model of a viscoelastic fluid. The calculations performed showed that the parameters of the fiber bundle produced depend on the method of forming used and on the local conditions in high-speed stretching, accompanied by oriented crystallization.

Introduction. The theoretical problems of the forming of single fibers have been widely covered in the literature. The main equations of motion of fibers within the framework of the Newtonian fluid model and the equations of heat exchange between the fibers and the medium were formulated for the first time in [1, 2]. More general equations for nonlinearly viscous fluids are derived by Entov and Yarin [3, 4]. Models of viscoelastic fluids were also used in studies of high-speed forming [5]. In [1, 2, 6–9], the equations obtained were used to perform numerical simulation of the process of stretching of single fibers for different schemes of forming and the main regularities of the process were established.

The main feature of the forming of fiber bundles is the hydrodynamic and thermal interaction of elementary fibers in the bundle. The process of forming of each filament depends on the location of the filament in the bundle and the conditions of interaction of the bundle with the medium. The calculations and experiments of [10, 11] show that during forming, a thermally and hydrodynamically stabilized flow region appears in the bundle. This region is in quasiequilibrium with the surrounding fibers and shows considerable conservatism with respect to external conditions (effects). Therefore, at the end of the forming zone, there is a marked difference in the parameters of separate fibers. In the present work, a mathematical model for process of forming of a fiber bundle is constructed and the main regularities of the process and the parameters of newly formed fibers are determined numerically.

1. Formulation of the Problem. The problem of forming of a fiber bundle consists of two groups of equations: the equations of motion and heat exchange between the bundle and the ambient medium and the equations of motion and heat exchange between elementary fibers with some determining parameters describing the process.

The first group includes the equations of convective heat exchange, [11, 12], which have the form

$$\varepsilon^{-1}\Big(u_1\,\frac{\partial u_1}{\partial x}+v_1\,\frac{\partial u_1}{\partial r}\Big)=-\varepsilon\,\frac{dp}{\rho dx}+R_U+\nu\,\frac{\partial}{r\partial r}\Big(r\,\frac{\partial u_1}{\partial r}\Big),\quad \frac{\partial(ru_1)}{\partial x}+\frac{\partial(rv_1)}{\partial r}=0; \tag{1.1}$$

$$\varepsilon^{-1}\rho c\Big(u_1\,\frac{\partial T_1}{\partial x}+v_1\,\frac{\partial T_1}{\partial r}\Big)=-\varepsilon^{-1}R_T+\lambda\,\frac{\partial}{r\partial r}\Big(r\,\frac{\partial T_1}{\partial r}\Big), \tag{1.2}$$

where (x, r) are cylindrical coordinates, u_1 and v_1 are the velocity components of the gas in the bundle in the x and r direction, T_1 is the gas temperature, ρ is the density, p is the pressure, ε is the porosity of the bundle

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$[\varepsilon = 1 - (r_f/r_\Delta)^2]$, ν is the kinematic viscosity, c is the specific heat, and λ is the thermal conductivity. The parameters R_U and R_T characterize the force and thermal interaction between the gas and the fiber:

$$R_U = (D/S)\tau_f, \qquad R_T = (D/S)q_f.$$

Here $D = 2\pi r_f$, $S = \pi r_\Delta^2$, r_f is the radius of a fiber, $r_\Delta = R_p N^{-1/2}$ is the radius of a cell, R_p is the radius of the bundle, N is the number of fibers, and τ_f and q_f are the friction and heat flux on the surface of a fiber. The analytical expressions for τ_f and q_f use the model of cells and the method of successive approximations. For gradient flow, the expression for τ_f and q_f in the first approximation have the form

$$\tau_f = \frac{\mu(\varepsilon U_f - u_1)}{r_f(1-B)\ln(r_\Delta/r_f)} - \left[1 - \varepsilon - \frac{\varepsilon B}{2(1-B)}\right]\frac{r_\Delta^2}{2r_f}\frac{dp}{dx},$$

$$q_f = \frac{\lambda}{r_f \ln(r_\Delta/r_f)}\,\frac{u_1(T_f - T_1)}{U_f(1-B) + (u_1 - \varepsilon U_f)c_0 + B_p(c_1 - \varepsilon^2 c_0/2)}, \tag{1.3}$$

$$c_0 = \frac{\ln(r_\Delta/r_f) - 1 + B}{(1-B)\ln(r_\Delta/r_f)}, \quad c_1 = \frac{B-1}{2} + \varepsilon - \frac{3}{4}\varepsilon B, \quad B = \frac{\varepsilon}{2\ln(r_\Delta/r_f)}, \quad B_p = \frac{r_\Delta^2}{4\mu}\frac{dp}{dx}.$$

The flow instability in a cell is taken into account by corrections of the second approximation. The expressions for τ_f and q_f in the second approximation are not given since they are cumbersome. Equations (1.1) and (1.2) describe the gas flow and the heat exchange in the fiber bundle, and for $\varepsilon = 1$ and $R_U = R_T = 0$, they describe the external region. Below, the superscript 2 refers to the flow parameters of the ambient medium. The interaction of the flows in the bundle and the ambient region is taken into account by the equalities of velocities, temperatures, friction stresses, and heat fluxes on the boundary of the bundle (at $r = R_p$), which, within the framework of the boundary-layer model [11, 13], have the form

$$u_2 = \varepsilon^{-1}u_1, \quad v_2 = v_1, \quad T_2 = T_1, \quad \mu\frac{\partial u_2}{\partial r} = \mu\frac{\partial u_1}{\partial r}, \quad \lambda\frac{\partial T_2}{\partial r} = \varepsilon\lambda\frac{\partial T_1}{\partial r}. \tag{1.4}$$

Expressions (1.4) must be supplemented by symmetry conditions on the axis of the bundle. For an exposed bundle, conditions for the external flow at infinity or conditions on the channel wall should be added. The equations of the second group, formulated in [14] using the mathematical model developed in [15], can be written as

$$Q\frac{dU_f}{dx} = \frac{d}{dx}(A\sigma_f) - 2\pi r_f\tau_f; \tag{1.5}$$

$$\sigma_f = \beta\frac{dU_f}{dx} - \beta\frac{U_f}{G}\frac{d\sigma_f}{dx}; \tag{1.6}$$

$$Qc_f\frac{dT_f}{dx} = 2\pi r_f q_f + QH\frac{d\Theta}{dx} + A\beta\Big(\frac{dU_f}{dx}\Big)^2 + 2\pi r_f q_r; \tag{1.7}$$

$$U_f\frac{d\Theta}{dx} = K_T K_\Delta(\Theta_* - \Theta), \tag{1.8}$$

where U_f and T_f are the velocity and temperature of the fibers, c_f is the specific heat of the polymer, A is the cross-sectional area of a fiber, Q is the flow rate of the polymer through the spinneret, σ_f is the stress, Θ is the degree of crystallinity, Θ_* is the degree of crystallinity in the equilibrium state, H is the latent heat of crystallization, G is the shear modulus, $q_r = \varepsilon_f\sigma(T_f{}^4 - T_\infty{}^4)$, σ is Boltzmann's constant, ε_f is the emissivity of the surface of a fiber, T_∞ is the temperature of the medium at infinity, and K_T and K_Δ are coefficients. Since the fiber bundle is a rather rarefied porous body, in calculations of radiation flows from the fiber surfaces, we shall ignore their mutual interaction.

Equation (1.5) is the equation of motion for a single thin fiber, Eq. (1.6) is the rheological equation of the fluid [15], Eq. (1.7) is the equation of heat exchange, and Eq. (1.8) is the phenomenological equation of crystallization, which corresponds to the Avrami equation with the exponent equal to unity. This choice of the exponent is based on theoretical and experimental studies of oriented crystallization [15–17]. The coefficient K_T depends only on temperature and determines the rate of crystallization in processes without stretching, the coefficient K_Δ depends on the birefringence parameter (BRP), and the coefficient Δn depends on the degree of stretching of the fiber and the molecular orientation of the polymer. According to [15], the BRP depends linearly on the internal stresses σ_f when the latter are low:

$$\Delta n = m\sigma_f. \tag{1.9}$$

System (1.1)–(1.9) is closed and completely determines the process of stretching of fibers from polymer melts with allowance for oriented crystallization. The system of equations of motion and heat exchange of the fibers (1.5)–(1.9) adequately describes the physical processes in the fiber, in particular, crystallization of the polymer during stretching of the fibers through the spinneret, which is essential to formation of the physical characteristics of the fibers.

The process of forming of fibers is conditionally divided into low and high-speed processes, depending on the rate of crystallization. High-speed forming typically produces fibers with high degrees of orientation of molecules and crystallinity. The occurrence of a local strain (neck) plays a special role in high-speed forming. The conditions of formation and development of a neck attracted the attention of researchers and was the subject of extensive research, for example, [6, 15]. In particular, in [15], various physical models are given and equations are formulated on the basis of kinetic and phenomenological concepts. One of these models, which is, in our opinion, the most complete, is described in the present paper. It can be used for a qualitative investigation of high-speed forming of fibers from polyethylene terephthalate (PETPH).

The experimental studies of [16–18] show that at low speeds of forming, PETPH has a low rate of crystallization with the formation of complex morphological modifications — crystallites [19]. High-speed forming ($U_f \sim$ 90–100 m/sec) gives rise to other structures [20, 21], which lead to strengthening of fibers. The degree of crystallinity in this case is about 0.4 and higher. Under such conditions, forming can be accompanied by the appearance of a neck in the region of fibers with low temperature. For this, as shown by the results of [15] and our calculations of forming of a single fiber, rather intensive cooling and high stress are required.

In forming of fiber bundles without using additional means of cooling (installation of blowers) thermal shielding results in different (from those for a single fiber) local conditions, which can substantially influence the orientation of molecular chains in the polymer. This model is intended to describe the main regularities of low-speed forming and to determine the possibilities of numerical simulation of the process of production of fibers with a high degree of orientation and crystallinity.

2. Calculation Results. Numerical simulation of the forming process is performed for three basic schemes of forming: in an open space without using blowers, in a shaft with blowing, and forming with stretching by an ejector. Calculations are performed for the following values of the determining parameters: the polymer density $\rho_f = 1356 - 0.5\,T_f$ kg/m^3, $c_f = 1260 + 2.52\,T_f$ J/(kg·K), $H = 121$ J/kg, $G = 10^8$ Pa, $\Theta_* = 0.4$, $\varepsilon_f = 1$, the initial radius of the bundle $R_p = 0.05$ m, the length of the forming zone $L = 2$ m; the longitudinal viscosity for PETPH was determined from the relation [15] $\beta = 0.725\exp[5260.0/(T_f + 273)](1 + 99\,\Theta)$.

Bundle in an Open Space. In forming of a fiber bundle in an open space, the ambient medium can be considered immovable. As a result, the boundary conditions for the equations of motion and heat exchange (1.1), (1.2) at infinity have the form $u_2(\infty) = 0$ and $T_2(\infty) = T_\infty$ (in the calculations, the temperature T_∞ was assumed to be equal to 20°C).

The problem of forming now is closed by the boundary conditions for the fibers, which, for a receiving device such as a roller rotating at constant rate, have the form

$$U_f(0) = U_{f0}, \qquad T_f(0) = T_{f0}, \qquad r_f(0) = r_{f0}, \qquad U_f(L) = U_L, \tag{2.1}$$

where the parameters with the subscript 0 are determined by the conditions on the spinneret, and U_L is rate of forming, which depends on the receiving device.

For Eq. (1.5), the boundary condition is specified at the end of the forming zone. This complicates the solution of Eqs. (1.1)–(1.9) since Cauchy problems are formulated for the stress, temperature, and degree of crystallinity of the fiber, and Eqs. (1.1) and (1.2) are parabolic equations. For the solution of boundary-value problem (1.5), (2.1), an iterative sequence of solutions of the Cauchy problems is constructed. As the iterative parameter we use the rheological force applied to the fiber at the cross section of the spinneret

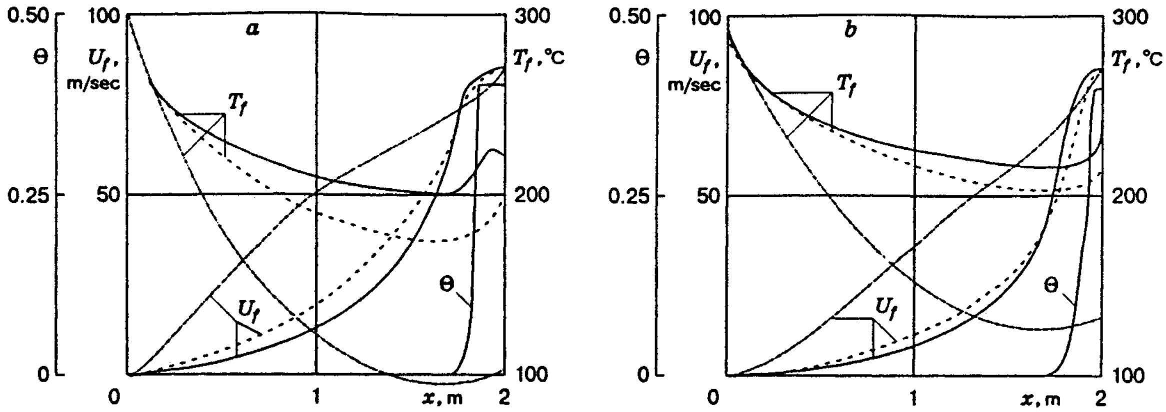


Fig. 1

$x = 0$. The iterative procedure of solution is as follows: the initial value of the rheological force F_{r0} [the rheological force $F_r = A\sigma_f$ and $F_{r0} = F_r(0)$] is assigned; for this value of F_{r0}, the problem of forming of a fiber bundle (1.1)–(1.9) is solved; the velocities of the fibers at the end of the forming zone $(u_L)_i$ are evaluated. If $|(u_L)_i/U_L - 1| > \alpha$ (i is the iteration number and α is the specified error of calculations), the value of F_{r0} is adjusted and the iterative process is repeated. If $|(u_L)_i/U_L - 1| < \alpha$, the repetitive process is completed. As calculations show, the number of iterations depends greatly on both the method of adjusting the value of the rheological force F_{r0} and on the features of the forming process. Thus, when the parameters of the outer and inner fibers differ greatly, for example, in forming of exposed bundles, the number of iterations required to attain the specified accuracy increases considerably. The average number of iterative cycles in calculations of the forming of an exposed bundle is about 50–60, and in forming in a shaft, it is 10–20.

Figure 1 shows curves of the velocity U_f, temperature T_f, and degree of crystallinity Θ of the fibers located on the s axis (solid curves), at half the radius w (dashed curves), and on the surface p of the bundle (dot-and-dashed curves). In the calculations, we used the following values: $U_{f0} = 0.5$ m/sec, $T_{f0} = 295$°C, and $r_{f0} = 0.000125$ and 0.00015 m (Fig. 1a and b, respectively). The number of fibers in the bundle $N = 100$, and the coefficient m is taken to be equal to $2.5 \cdot 10^{-9}$. It is obvious that for such parameters, the fibers of the bundle have different temperatures. As a result, the velocity of stretching of peripheral fibers with lower temperature grows faster than the velocity of inner fibers. This indicates that the thrust force exerted by the receiving device to the outer fibers is higher, and as a result, these fibers are in a more stressed state. However, crystallization proceeds only in fibers located in close proximity to the axis of the bundle. Qualitatively, the curves of the velocity and temperatures of fibers in the central part of the bundle differ only slightly, and jumps of temperature on these fibers can be clearly seen at the end of the forming zone. This is due to the fact that the degree of crystallinity Θ of such fibers rapidly reaches the equilibrium value $\Theta_* = 0.4$. The temperature of the fibers located on the surface of the bundle also undergoes a noticeable but fairly smooth rise at the end of the zone. This variation in the temperature is due not to the crystallization process in these fibers but to the fact that in a converging bundle, the outer fibers, while moving, fall in the region with a high temperature of the gas, which is in a quasiequilibrium state with the central fibers. The rise of the temperature of the fibers moving at half the radius of the bundle is observed at the end of the region considered. This is caused by both a decrease in the radius of the bundle and the beginning of orientated crystallization, which, in the scale of the figure, has not yet reached a marked value.

Bundle in a Shaft with Blowing. Forming in a shaft is accompanied by the supply of cooling air, which, together with the fiber bundle, moves along a channel of radius R_{ch}. On the wall of the shaft we assign $u_2(R_{ch}) = 0$, $T_2(R_{ch}) = T_w$, and $v_2(R_{ch}) = 0$, and the temperature on the channel wall T_w is assumed to be equal to 20°C. Boundary conditions (2.1) must be supplemented by the gas flow rate in the shaft. In our case (a simplified flow pattern), the velocity of air at the initial cross section is considered constant and equal to 4 m/sec, the initial conditions are the same as in the previous case, and the number of fibers $N = 100$.

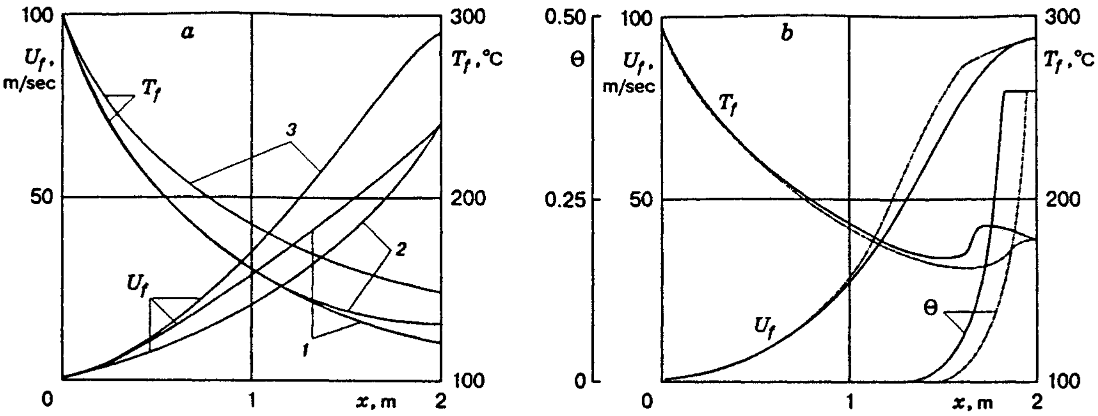


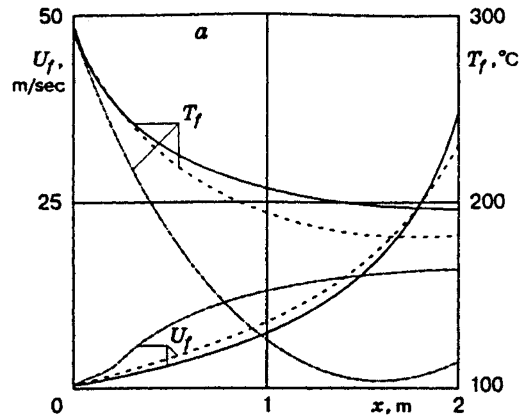
Fig. 2

Figure 2a gives curves of the velocities and temperatures for fibers on the axis of the bundle for three versions of calculation: $r_{f0} = 0.000125$ m and $U_L = 70$ m/sec (curves 1), $r_{f0} = 0.00015$ m and $U_L = 70$ m/sec (curves 2), and $r_{f0} = 0.000125$ m and $U_L = 95$ m/sec (curves 3). The spread of the fiber temperatures in the bundle is small, and, therefore, the velocities of the fibers located inside the bundle and on its surface differ only slightly (in the scale of the figure) from the velocities of the fibers on the axis of the bundle. From the calculation it follows that cooling of fibers in the shaft is more rapid and the temperature field is more uniform than in the previous case. It is obvious that in blowing shafts, the fibers are more uniform in their parameters, which is also confirmed by practice.

Curves 1 and 2 in Fig. 2 refer to results of a numerical simulation of low-speed forming. In this case, the temperature of fibers decreases smoothly, but for a thicker fiber, the temperature curve 2 is slightly above curve 1. The velocity curve for thicker fibers is under curve 1, which refers to thin fibers cooled at higher rate. Curves 3 correspond to a rather high speed of stretching of fibers, but the fiber temperature decreases rapidly and the fibers are not able to crystallize in this interval of motion.

A different picture is observed in forming of thicker fibers. Figure 2b shows (here and below, the notation of the curves is the same as in Fig. 1) curves of the velocity, temperature, and degree of crystallinity for $r_{f0} = 0.00015$ and $U_L = 95$ m/sec. Since, in this case, the temperature of fibers decreases more slowly, the fibers are under conditions that favor fast crystallization of the polymer. The abrupt jumps of temperature at the end of the forming zone and sharp rises in the degree of crystallinity can be clearly seen. An important feature of the process considered, as compared to the process for a rapidly cooled single fiber [15], is that in both exposed bundles and bundles moving in a shaft, crystallization proceeds at higher temperatures and, according to experimental results, at rather low values of the BRP Δn (in our calculations for low-temperature stretching of a single fiber, the BRP reached values of about 0.08–0.1, and, for the cases considered, $\Delta n \sim 0.03$–0.04). It should be noted that, despite the slight difference in temperature and velocity between the central and peripheral fibers before crystallization, the process of oriented crystallization begins at different distances from the spinneret and results in layering of the curves. This indicates the high sensitivity of oriented crystallization to the forming conditions.

Aerodynamic Forming. In contrast to the two previous schemes, in which the speed of stretching of fibers is specified, the forming in this case is implemented by means of an ejector. The technological, physical, and mathematical aspects of the problem were studied in a number of papers, for example [9, 22–24], where the features of aerodynamic forming are considered, a mathematical formulation of the problem is given, and the main regularities are established. Analysis of the problem shows that the boundary condition for the fiber at the end of the forming zone is the equality $F_r = F_{\rm fr}$, where $F_r = F_i + F_f + F_{r0}$ is the rheological force acting on the jet directly ahead of the ejector, F_{r0} is the rheological force in the cross section of the spinneret, F_i is the force of inertia, F_f is the force of friction a fiber in the medium, and $F_{\rm fr}$ is the force of friction of the fiber in the ejector. Ignoring the direct interaction of the fibers with each other and with the wall



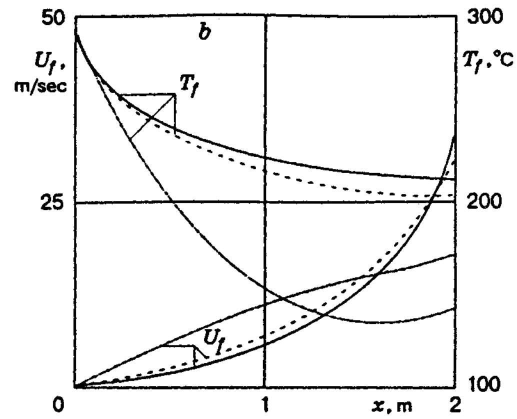


Fig. 3

at random contacts, we can write the expression for F_{fr} as [15] $F_{fr} = 2\pi r_f l \rho c_f (U_{fr} - U_f)^2$, $c_f = 0.5\,\mathrm{Re}^{-0.61}$, $\mathrm{Re} = 2r_f(U_{fr} - U_f)/\nu$ (l is the length of the ejector). It is also assumea that, according to [9], because of rapid cooling, the radius of a fiber in the ejector varies only slightly, owing to which it can be considered constant.

Figure 3 shows the velocity and temperature distributions for fibers in exposed bundles formed by means of an ejector of length $l = 20$ cm in which the gas velocity is $U_{fr} = 200$ m/sec; the calculations were performed for $N = 100$, $r_{f0} = 0.000125$ m (Fig. 3a), and $r_{f0} = 0.00015$ m (Fig. 3b). From the figure it follows that when the fibers move, the temperature of inner fibers decreases smoothly and reaches a local level that is in quasiequilibrium with the medium. As in the problem for an exposed bundle, a characteristic feature of this problem is the considerable difference in temperature between surface and inner fibers. Since the temperature of outer fibers is well below that of the central fibers, the velocity of the outer fibers at the ejector is approximately twice lower than the velocity of hot fibers. The small bend of the velocity curves for the outer fibers observed in Fig. 3 is caused by the increase in their temperature due to entry into the hot gas region.

In conclusion, the following should be noted. The mathematical model constructed makes it possible to calculate the processes of forming of bundles of fibers under different conditions. The solutions obtained showed the qualitative regularities of the motion and temperature distribution of the fibers formed. The calculation of low-speed forming does not involve considerable mathematical difficulties. Equations (1.1)–(1.9) are solved numerically by the method developed in [25] using the Crank–Nicholson finite-difference scheme. The convergence of the solutions with an appropriate choice of the initial conditions indicates stability of the adopted iterative process. The dependence of the final parameters of the fibers on the parameters of the mathematical model can be significant, but it is well controllable during solution.

For high-speed forming, which involves a change in the molecular structure, accompanied by high dynamic and temperature stresses resulting in jumps of temperature and local elongations, the computations become more difficult. In this case, use of the extrapolation method of [26] to integrate the one-dimensional equations (1.5)–(1.9) simplifies the solution considerably. It is worth noting, however, that the model of orientated crystallization of [15], in the opinion of its authors, has a qualitative nature and requires further studies. Our calculations of the forming of both single fibers and bundles indicate that the process of oriented crystallization is extremely sensitive to external conditions (see Fig. 2b) and to some parameters of the mathematical model. According to this, the model should be refined using results of experiments with careful observance of experimental conditions in order to provide quantitative agreement with real values.

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