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NUMERICAL MODELING OF HEAT TRANSFER IN A BUNCH OF CRYSTALLIZING MOVING FIBERS

V. I. Eliseev, Yu. P. Sovit, and
L. A. Fleer

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A mathematical model of heat transfer in a bunch of crystallizing polymer fibers is suggested and a numerical analysis of fiber stretching in an open medium and in an axisymmetric channel is carried out.

One of the important problems in the production of synthetic fibers is determination of the dependences between the molding conditions and the internal processes in the fibers that determine the structure and quality of the fibers. Among the physical phenomena occurring in a melt in molding, crystallization plays an essential role in the development of the fiber properties. An interdependence is observed among the processes of crystallization, heat transfer, fiber stretching, and degree of orientation of the polymer molecules. Account for these phenomena and determination of their influence on the crystallization process represent a rather complicated problem because of the absence of complete kinetic equations that take into consideration the variety of molecular and supermolecular structures of polymers.

Different variants of mathematical modeling of the crystallization of polymer materials are known – from the simple Avrami models to more complicated ones described by integrodifferential equations [1–4]. Among this diversity a mathematical model [2, 3] that is distinguished by its simplicity and is represented by the equation for the degree of crystallinity

$$\frac{d\vartheta}{dt} = K(T)(\vartheta_* - \vartheta), \tag{1}$$

where K depends on the temperature, attracts attention. For processes involving fiber stretching these quantities depend on the molecular orientation, which is determined by the internal stresses in the fibers. A number of works, whose results are reported in monograph [5], are devoted to the establishment of such dependences and the possibility of their use for calculating the crystallization of single threads. In the present work these developments are used to construct a mathematical model of molding a bunch of fibers with account for the process of polymer crystallization. Results of numerical calculations of real schemes of production of complex fibers are reported.

Formulation of the Problem. For an axisymmetric bunch with radius $R_b(x)$ consisting of N elementary fibers with radii $R_{fib}(x)$, within the framework of the model of a filtration flow in a porous body and a boundary layer the basic equations of convective heat transfer are as follows [6, 7]:

$$\varepsilon^{-1}\left(u_1\frac{\partial u_1}{\partial x} + v_1\frac{\partial u_1}{\partial r}\right) = -\varepsilon\frac{\partial p}{\rho dx} + \nu\frac{\partial}{r\partial r}\left(r\frac{\partial u_1}{\partial r}\right) + R_U,$$

$$\varepsilon^{-1}\rho c\left(u_1\frac{\partial T_1}{\partial x} + v_1\frac{\partial T_1}{\partial r}\right) = \lambda\frac{\partial}{r\partial r}\left(r\frac{\partial T_1}{\partial r}\right) + \varepsilon^{-1}R_T, \tag{2}$$

$$\frac{\partial(ru_1)}{\partial x} + \frac{\partial(rv_1)}{\partial r} = 0,$$

where R_U and R_T characterize the force and heat interaction between a gas and a fiber:

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$$R_U = \frac{2\pi R_{fib}}{\pi R_\Delta^2}\tau_{fib}, \quad R_T = \frac{2\pi R_{fib}}{\pi R_\Delta^2} q_{fib}, \quad \varepsilon = 1 - (R_{fib}/R_\Delta)^2.$$

Analytical expressions for τ_{fib} and q_{fib} are obtained in [6, 7].

A zone of uniform gas flow is adjacent to the bunch on its outer side. The equations of motion and heat transfer in this zone are of the same form as (2) at $\varepsilon = 1$ and $R_U = R_T = 0$. Similarly to [6, 7], conjugation conditions are set for the filtration parameters and quantities in the external region at the bunch boundary. In order to close the system of equations (2), it is necessary to determine the distributions of radii, velocities, and temperatures of the fibers in the bunch volume. Using the Maxwell liquid model [5], we write the equation of motion and the constitutive equation for a polymer fiber:

$$Q\frac{dU_{fib}}{dx} = \rho q S + \frac{d}{dx}(S\sigma) - 2\pi R_{fib}\tau_{fib}, \tag{3}$$

$$\sigma = \beta\frac{dU_{fib}}{dx} - \beta\frac{U_{fib}}{G}\frac{d\sigma}{dx}. \tag{4}$$

Calculations of molding of single threads show that the force caused by the thread's own weight is insignificant. Integrating Eq. (3) without this force, we arrive at the expression

$$S\sigma - QU_{fib} = F + 2\pi\int_0^x R_{fib}\tau_{fib}dx, \tag{5}$$

which is used below in calculations for the specified pulling force F. As the kinetic equation describing the crystallization process of polymer fibers, we use the expression [5]

$$U_{fib}\frac{d\vartheta}{dx} = K_T K_\Delta(\vartheta_* - \vartheta), \tag{6}$$

which differs from Eq. (1) by the fact that $K = K_T K_\Delta$. The parameter K_T depends only on the temperature and determines the rate of crystallizarion without stretching, and the second cofactor depends on the birefringence, which is a measure of fiber stretching and molecular orientation of the polymer. For polyethyleneterephthalate (PETP) the dependences K_T, K_Δ are as follows [5]:

$$K_T = \exp\left[9.34 - \frac{683}{T - 43} - \frac{4.53\cdot 10^5}{(T + 273)(300 - T)}\right], \tag{7}$$

$$K_\Delta = \exp\left\{\frac{1.2\cdot 10^6}{(T + 273)(300 - T)} \times \left[1 - \frac{1}{1 + 160(\Delta n)^2 (T + 273)/(300 - T)}\right]\right\}. \tag{8}$$

According to [2, 5] at low internal stresses of stretching σ the birefringence depends lineary on it, i.e.

$$\Delta n = m\sigma, \tag{9}$$

Here the stress must be determined from the equations for fiber motion (4), (5).

We supplement the presented system with the heat transfer equation for a single thermally thin thread with account for the phase heat release upon crystallization:

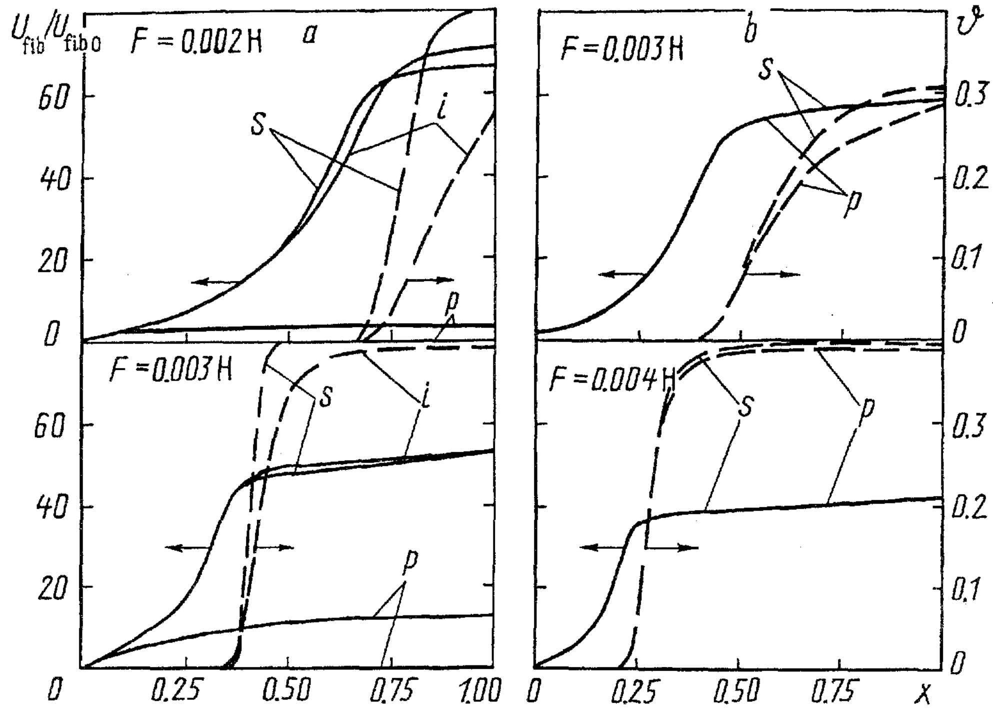

Fig. 1. Distributions of velocity and degree of crystallinity of fibers along the zone of molding of a bunch in an unbounded medium (a) and in a column (b): solid lines, velocities; dashed lines, degreeof crystallinity; s, bunch axis; i, 1/2 radius; p, bunch surface. x, m.

$$Qc_{fib}\frac{dT_{fib}}{dx} = 2\pi R_{fib}q_{fib} + QH\frac{d\vartheta}{dx}. \tag{10}$$

Equations (4)-(10) describe the problem of moulding a single crystallizing thread. The shear stress τ_{fib} and the heat flux q_{fib} on a fiber surface determine the external conditions of molding. We determine these quantities by solving system of equations (2). Simultaneously solving the problem of molding (4)-(10) for the calculated τ_{fib} and q_{fib} we may calculate the parameters of the fibers formed in the bunch volume. To test the crystallization model under consideration, we predicted the molding process for a single fiber by using criterial relations for friction and heat transfer [5]. Results of the calculations representing the distributions of temperatures, velocities, degree of crystallinity, and birefringence along a molding section were in satisfactory agreement with the data reported in [5]. This confirmed that the above equations are adequate for the mathematical model used in [5].

Open Bunch. An open bunch means a bunch of fibers moving from a spinneret surface to a receiving unit in unrestricted space with known distributions of velocities and temperatures at infinity. In this case the initial system of equations is supplemented with the boundary conditions at infinity $u_2(\infty) = 0$, $T_2(\infty) = T_0$, and the governing parameters are as follows: $R_{fib\,0} = 0.05$ m; $R_{b\,0} = 0.000125$ m; $N = 100$; $U_{fib\,0} = 0.5$ m/sec; $T_{fib\,0} = 290$ and 280°C; $\rho_{fib} = 1356-0.5T_{fib}$ kg/m^3; $c_{fib} = 1260 + 2.52T_{fib}$ J/(kg·K); $H = 50{,}300$ J/kg; $\vartheta_* = 0.4$; $m = 5.3\cdot10^{-9}$ Pa^{-1}. The longitudinal viscosity for PETP is determined from the following relation [5]:

$$\beta = 0.725 \exp\,[5260.0/(T_{fib} + 273)]\,(1 + 99\,\vartheta)\,.$$

System of equations (2) together with the equations of motion and heat transfer of a homogeneous gas was integrated numerically by the method of [8]. To integrate Eqs. (4)-(6), (10), the extrapolation method [9] was used.

Figures 1a and 2a present calculation results for $N = 100$ and different values of the pulling force F. As an analysis of the results shows, for an open bunch the processes of fiber pulling and crystallization depend almost

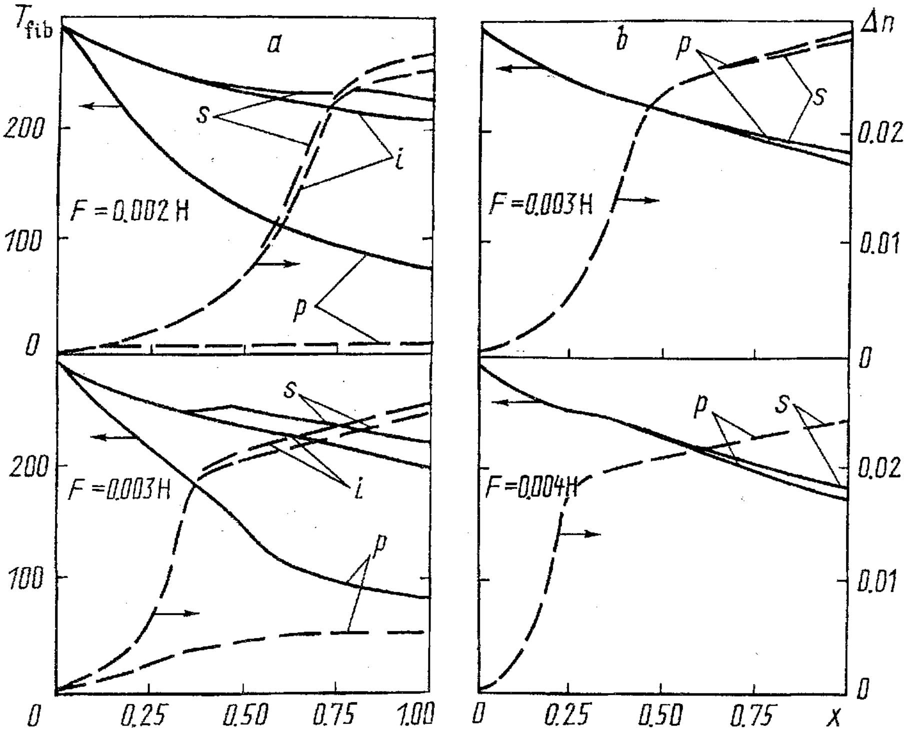

Fig. 2. Distribution of temperature and birefringence of fibers along the zone of molding of a bunch in an unbounded medium (a) and in a column (b): solid lines, fiber temperature; dashed lines, birefringence. T, °C.

completely on the hydrodynamic interaction between the system of fibers and the cooling medium. Thus, as a result of formation of a flux in the bunch volume intense air ejection from the outer to the central regions occurs, which causes quite rapid cooling of the outer fibers. As a consequence, the birefringence and the degree of crystallinity for them become close to zero and the velocity of motion rapidly attains its limiting value due to a substantial increase in the longitudinal viscosity of the polymer. After becoming cooled on the initial section, the central fibers reach a practically thermostabilized zone with a high temperature level. Here substantial stretching of the fibers is observed. As a result, the birefringence undergoes a rapid increase, which leads to intense crystallization of the polymer. The phase heat released here causes small temperature jumps in the central threads. Owing to an increase in the longitudinal viscosity the velocity of the fibers becomes almost constant along the molding space after crystallization. At a distance from the bunch center the fiber temperature decreases and crystallization proceeds more smoothly, and therefore in the middle of the bunch, fibers with a higher degree of stretching, compared to the center, may be obtained.

The results presented allow a judgment about the influence of the pulling force F on the molding and heat transfer of a complex thread. As is seen from the figures, an increase in F results in more pronounced growth of the birefringence, which displaces the onset of crystallization upward along the thread. Simultaneously, the temperature of the onset of crystallization rises, the velocity increases sharply, and, as a consequence, the released heat causes more abrupt jumps in the fiber temperatures. In fiber stretching, the influence of the pulling force is manifested in a somewhat paradoxical form: with an increase in the pulling force the final velocity of the crystallizing fibers in the bunch decreases. This is associated with the influence of the degree of crystallinity on the longitudinal viscosity – β increases sharply with an increase in the degree of crystallinity. Therefore in order to obtain well-stretched threads with a small final diameter, it is necessary to increase the heat transfer rate while increasing the pulling force. Calculations performed for a lower initial temperature have shown (these results are not given in the figures) that the onset of crystallization is displaced downward along the flux and occurs at lower temperatures. Changing the quantity of fibers in the bunch does not lead to marked differences in the described regularities of the behavior of the temperatures, the birefringence, and the degree of crystallinity.

Bunch in a Channel. For numerical modeling of the crystallization of a fiber bunch in a blown column the system of equations (2), (4)-(10) was supplemented with the boundary conditions on the column wall $u_2(R_c) = 0$, $T_2(R_c) = T_w$. Calculations were made for the following parameters: $R_c = 0.1$ m; $Q_g = 0.063$ m^3/sec; $T_w = 20^oC$; $F = 0.003$ and 0.004 N. The remaining quantities were the same as in the case of an open bunch. Calculation results are given in Figs. 1b and 2b. As is seen from the behavior of the fiber temperatures, heat transfer is more intense in the case of the adopted relations than in an open channel. As a result, the onset of crystallization is shifted farther downstream. Since there is practically no temperature drop over the bunch thickness, the crystallization proceeds with virtually the same intensity for the all fibers. The temperature of the onset of crystallization is somewhat lower, the process itself proceeds at a lower rate, and there are no temperature jumps. The velocity distribution of the fibers is indicative of the uniformity of the conditions in the bunch. An increase in the pulling force exerts a weak influence on the heat transfer but, as in the case of open cooling, it displaces the onset of crystallization upstream. The distributions of birefringence and the degree of crystallinity become steeper and an isothermal zone develops in the temperature distributions. The displacement of the crystallization point upward also causes a marked increase in the final diameter of the obtained fibers.

The problems discussed are a first approximation to a solution of the complete problem of molding of complex threads, for which the pulling force distributions over the bunch radius must be corrected proceeding from the boundary conditions at the end of the molding zone. On the whole, the calculations performed have shown the sensitivity of the crystallization process to the conditions under which it proceeds and the difference in the regularities of motion and heat transfer of threads in open bunches and in bunches moving in a column. When the suggested model is used in practice, it is necessary to refine the corresponding kinetic dependences in each particular case.

NOTATION

x, r, coordinate system; u, v, velocities; ρ, density; p, pressure; T, temperature; c, heat capacity; ν, kinematic viscosity; λ, thermal conductivity; ϑ, degree of crystallinity; Δn, birefringence; H, heat of the phase transition; ε, bunch porosity; σ, stress of fiber stretching; τ_{fib}, q_{fib}, friction and heat flux on the fiber surface; S, cross-sectional area of the fiber; Q, polymer consumption per spinneret; R_{fib}, fiber radius; R_b, bunch radius; R_c, column radius; F, force; β, longitudinal viscosity; G, shear modulus; N, quantity of fibers in the bunch. Subscripts: fib, fiber; ∞, outer medium; w, channel wall; 0, initial cross section; 1, filtration parameters; 2, zone of uniform flow.

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