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Simulation of Diffusion in Bicomponent Fibers of the Core-Cladding Type

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Polycomponent chemical fibers are widely used to modify properties of materials. Bicomponent fibers of the core-cladding type (C/C type) are among them [1]. In manufacturing a bicomponent fiber, the proper choice of polymeric components is of great importance. The components should be thermodynamically compatible and provide good cladding-to-core adhesion. This process may be described in terms of the theory of diffusion [2]. Therefore, investigation of the interdiffusion of the components of a C/C fiber may be useful for calculating the length of the transition zone. To a large extent, this zone determines the strength of cladding-to-core adhesion as well as the mechanical and thermal stability of the fiber.

In this paper, we suggest a mathematical model of diffusion in bicomponent fibers and ascertain the relationship between the length of the transition zone and the parameters of the technological process of fiber formation from melt. The model is based on the analysis of the physical mechanism of diffusion and the following assumptions:

(1) In accordance with the experimental data of [2], the length of the diffusion zone is a few microns. It is much less than the fiber radius, which is approximately one millimeter. Therefore, diffusion flows are supposed to be localized along the fiber radius in the contact zone and equal to zero in the center and on the surface of the fiber. Due to this assumption, we can restrict our consideration to diffusion in two semiinfinite media with a plane interface.

(2) The main part of the transition zone is formed during the time needed for the thread extruded through a spinneret to solidify. It should be taken into account that the diffusivity of the melt is two or three orders higher than that of a solidified fiber [2].

(3) The dependence of the diffusivity on the temperature in the diffusion zone [2] should also be considered because fiber formation is an essentially nonisothermal process.

(4) The beat-transfer problem is considered in its axially symmetric one-unidimensional formulation because a fiber may be viewed as a homogeneous cylinder with a radius much less than the length of the formation zone. The thermal characteristics of the fiber components differ insignificantly.

Interdiffusion of the components takes place in the fiber. The resulting direction of diffusion depends on the diffilsivities of the components. Without loss of generality, we can consider diffusion from the core material into the cladding. The equations of diffusion in the core are

$$\frac{\partial C_s}{\partial t} = \frac{\partial}{\partial x}\left(D_s\left(T_g\right)\frac{\partial C_s}{\partial x}\right) \quad , \quad x < 0;$$
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\left(T_g\right)\frac{\partial C}{\partial x}\right) \quad , \quad x > 0; \qquad (1)$$

The equation describing the diffusion of the cladding material into the core for C = C_0 and D= $D_0(T_g)$ can be written in a similar way. The x-axis is directed along the fiber radius, and the point $x = 0$ coincides with the coordinate $r = R$ of the core-cladding interface. If the direction of the coordinate r coincides with the direction of the x-axis, then $x = r - R$. However, these quantities have different scales because of the difference of at least five orders between diffusivity and thermal diffil-sivity. Heat transfer in the cylinder can be described by the equation

$$\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(a(T)r\frac{\partial T}{\partial r}\right) \quad , \quad r \in \left(0, R_0\right). \qquad (2)$$

The initial conditions at $t = 0$ are

$$T(r,0) = T_n(r); \qquad (3)$$

$$C(x,0) = 0 \, for \, x > 0; \qquad (4)$$

$$C_s(x,0) = 1 \, for x < 0; \qquad (5)$$

The boundary conditions are

$$-\lambda(T)\frac{\partial T(R_{0,}t)}{\partial r} = \alpha\left[T(R_{0,}t) - T_s(t)\right]\Big|_{r=R_0}; \qquad (6)$$

$$\left.\frac{\partial C}{\partial x}\right|_{x\to\infty} = 0 \qquad (7)$$

at the outer surface of the fiber for $r = R_0$ and $x \to +\infty$;

$$C(x,t) = C_s(x,t), \tag{8}$$

$$D(T_g)\frac{\partial C(x,t)}{\partial x} = D_s(T_g)\frac{\partial C_s(x,t)}{\partial x}\bigg|_{X=0} \tag{9}$$

at the core-cladding interface for $x = 0$; and

$$\frac{\partial T(r,t)}{\partial r}\bigg|_{r=0} = 0; \tag{10}$$

$$\frac{\partial C_s}{\partial x}\bigg|_{x\to-\infty} = 0. \tag{11}$$

in the center of the fiber for $r = 0$ and $x \to -\infty$

To solve the nonlinear system of equations (l)-(ll), we used an implicit scheme of the finite-difference method [3]. The algebraic system of equations was linearized by iterations [3], whose number in calculations did not exceed three.

For numerical simulation by the model suggested, we have to know the coefficients of heat and mass transfer. We assume that the core-into-cladding diffusivity is equal to the diffusivity of the core, $D = D_s$. The temperature dependence of diffusivity is taken as $D \approx exp(- I/T)$. The values of D are taken from [2]. First, we have to find the diffusivity at constant temperature and then determine its dependence on the temperature T_g.

The diffusivity $D= 4.09 \times 10^{-13}\ m^2 s$ for $T= 200°C$ is obtained by the method of discrepancies [5] using the experimental distributions of concentration with the coordinate given in [2]. The temperature dependence of diffusivity found from the data for a variety of polymers presented in [2] is

$$D(Tg)=D_c exp[-3843/(Tg+273)], \tag{12}$$

where $D_c= 1.38 \times 10^{-9}\ m^2/s$ in the temperature range $T_g = 100$- $250°C$. The diffusivity was calculated for $T_g = 200°C$. According to (12), when T_g is reduced by $100°C$, the diffusivity decreases by one order.

The values of thermal conductivity and thermal diffusivity for polymethyl methacrylate necessary for solving the problem of heat transfer were taken from [6],

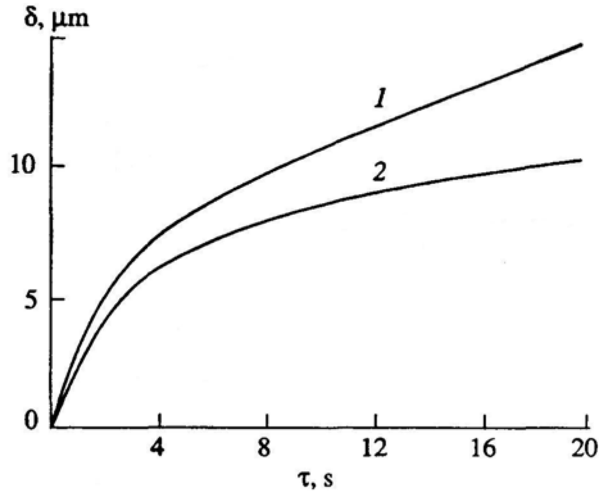

Fig. 1. Time dependence of the length of the diffusion zone: (7) $D = const$; (2) with allowance made for $D(T_g)$.

with their temperature dependences taken into account. The heat-transfer coefficient was determined through numerical simulation. It was found to be equal to $\alpha = 40 W/(m^2K)$ for $R = 5 \times 10^{-4}\ m, R_0 = 10^{-3}\ m$, and $T_g = 573\text{-}383K$

The diffusion zone is defined as a region on the interface between the fiber components where the variation of concentration is more than 5% of the initial concentration. To calculate the length of the diffusion zone S, we obtained the system of transcendental equations

$$\begin{aligned} &C_s\left(x_{1,}\, t\right) = 0.95\ for\ x < 0 \quad ; \\ &C\left(x_{2,}\, t\right) = 0.05\ for\ x > 0 \quad ; \\ &\delta = x_2 - x_1 \quad . \end{aligned} \tag{13}$$

The variation of the diffusion zone (Fig. 1) in time was determined by (13). The adhesion of the components of a C/C fiber may bejudged from $\delta(t)$ [4]. Comparison of results calculated at a constant diffusivity and with allowance for temperature dependence (12) showed that the length of the diffusion zone was reduced from $\delta = 15\ \mu m$ to $\delta = 10\ \mu m$ in $t = 20\ s$ due to the cooling of the fiber.

To find the relationship between the length of the transition zone and the parameters of the technological process of nonisothermal formation, we used the suggested mathematical model and investigated the dependence of the length of the diffusion zone δ on the heat-transfer coefficient α and the temperature T_s of the medium. The results of numerical simulation are given in Fig. 2.

The length of the diffusion zone may be estimated by solving a similar linear problem of mass transfer

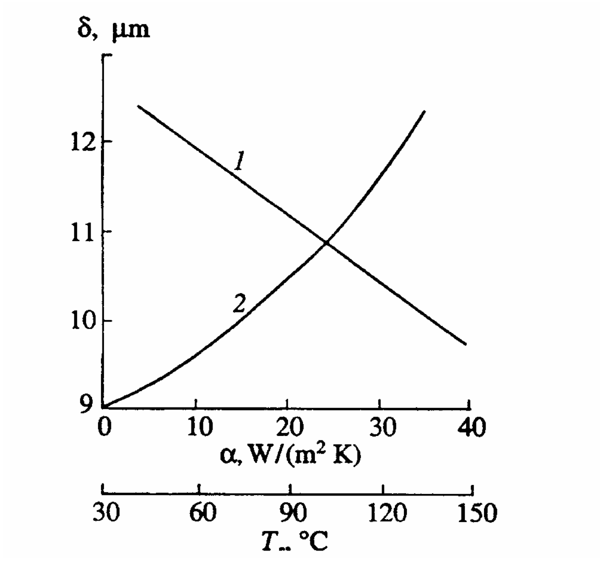

Fig. 2. Length of the diffusion zone as a function of (7) the heat-transfer coefficient and (2) the temperature of the ambient medium at $t = 20s$.

(for $D = const$) [7]. The solution is the error function of the argument

$$\xi = x/2\sqrt{D\tau}; \tag{14}$$

Due to the monotony of this solution, the diffusion zone corresponds to the interval $|\xi| < 1.4$. This fact can be used to estimate 5. In (14), we have to set $x = 0.58$ because the diffusion zone is both in the core and the cladding. The constant D should be replaced by

$$D = \frac{1}{\Delta T_g} \int_{T(\tau)}^{T(0)} D(T)dT \quad , \tag{15}$$

which is the diffusivity averaged over the temperature in the boundary zone *Tg* varying in time *T*.

The following expression is obtained for the length of the diffusion zone:

$$\delta = 5.6\sqrt{D\tau} \quad , \tag{16}$$

which gives $\delta = 11.2\ \mu m$ for the values chosen for numerical simulation. This result checks well with the length of the diffusion zone calculated within the nonlinear model and equal to $14.2\ \mu m$.

Note that an increase in the length of the diffusion zone leads, as a rule, to stronger core-to-cladding adhesion. Therefore, in accordance with the model suggested, increasing the residence time of a fiber in a high-temperature zone is desirable. For this purpose, it is advantageous to arrange heating chambers in the formation zone or anneal a bicomponent fiber after its formation.

NOTATION

a - thermal diffusivity, m^2/s;

C, C_s - relative concentration of the core material at a point x and time t *for* $x > 0$ *and* $x < 0$,

D, D_s - diffusivity of the core material at a point x and time t for $x > 0$ and $x < 0$, m^2/s;

R, R_0 - radii of the core and the fiber, m;

T - temperature of the fiber, °C;

T_n - initial temperature of the fiber at $t = 0$, °C;

T_g - temperature of the diffusion zone, °C;

T_s - temperature of the ambient medium, °C;

α - heat-transfer coefficient of the fiber, W/(m K);

λ - thermal conductivity, W/(m K);

δ - length of the diffusion zone, m.

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