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MODELING OF SURFACE MODIFICATION OF SEWING THREAD

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Second-order regression polynomial mathematical models describing the characteristics of modification of sewing thread by application of coatings were constructed. The adequacy of the regression equations makes the proposed method a good tool for analysis of multifactor mechanisms with a large set of experimental data.

Giving polymeric articles used in medicine, biotechnology, veterinary medicine, and cosmetology biocompatibility is an extremely important and interesting problem for chemists, biologists, and medical personnel. Biocompatibility is a set of properties that ensure the absence of any negative reaction of biological objects on contact with polymeric implants. It was previously believed that biocompatibility is determined by the inertness and hydrophoby of the materials [1], but recent studies [2, 3] showed that the surface of an implant should have a certain balance of hydrophilic-hydrophobic and other properties to stimulate adhesion of cells but prevent thrombogenesis and adhesion of bacteria. Ideally, the surface of the implant should thus be a unique smart material that recognizes different cells and is adequately reconstructed. Such materials cannot be created without a detailed study of the complex and multifactor correlations of the structure, composition, external conditions, and properties conducted with modern computers and software.

Modern sewing materials should have antimicrobial activity, stability in sterilization, low capillarity and porosity, high knot strength and tying capacity, and atraumaticity. Their color should differ from the color of the fabrics sewn and when drugs are incorporated in them, they should have a lasting action. Thread with a "core—shell" structure, obtained by application of a complex twisted or woven thread with a drug-filled coating made of a biocompatible polymer on the surface, most fully satisfies the above requirements [4-6]. The coating reduces the capillarity and by giving the thread the structure of a pseudomonofilament, decreases its traumaticity without worsening the capacity to tie surgical knots.

We used mathematical modeling of the effect of the process parameters of modification of synthetic fibres by applying a biocompatible polymer coating on their properties to solve the problem of creating sewing thread with improved properties. Polyhydroxybutyrate (PHB) — a promising polymer of microbiological origin — is such a biocompatible polymer. PHB is soluble in highly volatile solvents (methylene chloride, chloroform), melts at 170°C without decomposing, and forms strong fibres in melt spinning [7]. However, fibres and films spun from solutions are characterized by high strength. Since production of this polymer is in the organizational stage, we conducted mathematical and experimental modeling of the effect of the conditions of applying the coating from polymer solutions on the properties of the fibre obtained, anticipating the introduction and use of PHB for modifying fibres made of synthetic polymers. Cellulose triacetate in the form of equiviscous (or equiconcentrated) solutions in methylene chloride was also used together with PHB in the stage of testing the laboratory setup and modeling the process. Polycaproamide (PCA) and Ftorlon fibres, widely used in domestic medical practice, were the initial sewing thread (Table 1).

The polymer-modifier was applied to the fibre on a setup (Fig. 1) that impregnated the fibre with the modifying solution, and the excess solution was squeezed out with the removable rings and dried in a hot air stream under tension. To select the optimum modification conditions, we tested 20 regimes for application of the polymer on the fibre. The concentration of polymer in the solution, squeezing, and the fibre speed were varied, and the effect of these parameters on the linear density, strength, and elongation at break of the bicomponent thread obtained was investigated.

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TABLE 1. Physicomechanical Indexes of the Initial Fibres

Fibre	T, tex	P_r, cN	σ, cN/tex	ε, %
Ftorlon	16.3	528	32.4	9.5
PCA	27.6	1027	37.2	13.2

Notation: T — linear density; P_b — breaking load; P_r — relative breaking load; ε — elongation at break.

TABLE 2. Plan Matrix of the Second-Order Nonlinear Model of a Three-Factor Experiment

Input parameters	Concentration of polymer, %	Thread speed, m/min	Number of detachable rings
Basic level	3	15.5	4
Variation step	1.2	5.7	1
Lower level	1.8	9.8	3
Higher level	4.2	21.2	5
Star points			
+ 1.68	5	25	6
– 1.68	1	6	2

The selection of the range of variation of these modification parameters was based on preliminary experiments to establish the "star points" — the critical values below or above which the polymer is applied to the fibre to no purpose. A shortage of polymer binder was observed at the lowest concentration of the modifying solution and was reflected in the morphological characteristics of the sewing thread. It was inhomogeneous and had sites with poorly glued monofilaments. At a concentration above 5%, bulges and nubs of the polymer modifier formed in the thread.

The range of variation of the speed conditions was found between the minimum rate of movement of the fibre (6 m/min) at which the polymer solution could not dry on the fibre inside the cylinder and the maximum rate (25 m/min) at which breaks did not form for the complete time of operation of the setup.

The star points were selected with all other parameters being equal. The step and numerical values of the other levels of variation (Table 2) were determined according to the recommendations on design of experiments [8]. A second-order nonlinear model of the reciprocal effect of the conditions of application of the coating on the optimization parameters was selected in the calculations, since it most adequately described the results of modification.

The samples of the fibres before and after reaction with the modifying solution were investigated by electron microscopy in a Joel JSM-5300 LV scanning electron microscope.

A sample of the initial Ftorlon fibre is shown in Fig. 2, where the filaments are clearly visible, and a sample of modified Ftorlon fibre with a coating of 5% polymer solution is shown in Fig. 2*b*. Note the formation of an almost continuous layer of modifying polymer in Fig. 2*b*, while treatment with less concentrated solutions only causes partial gluing of the monofilaments. The coating thickness estimated with the photograph was approximately equal to 3 μm, which correlates well with the value of 2 μm (Table 3) calculated with the increase in the thickness of the fibre. It is thus possible to conclude that it is necessary to apply a coating from solutions with a minimum concentration of 5% must be applied for formation of a pseudomonofilament with a core—shell structure.

The physicomechanical characteristics of the initial and bicomponent fibres were investigated on a Fritz Heckert FP 10/1 tensile-testing machine (Germany) at room temperature (initial sample length of 100 mm, stretching rate of 120 mm/min). The absolute and relative breaking load and relative elongation at break were measured.

The mathematical analysis of the results of the experiment and modeling of the manufacturing process were conducted with Mathcad-12 software, which also allows determining the regression function of the dependence, for example, of the linear density (Z) on the concentration (C) and takeup rate of the fibre in the output pack (S). Determination of the coefficients of the

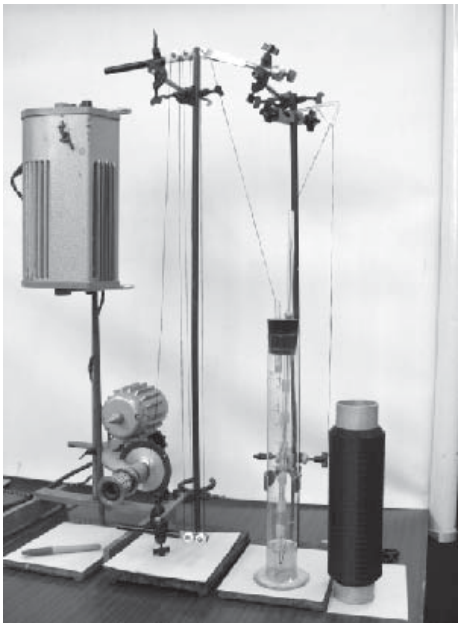

Fig. 1. Setup for application of coating to thread.

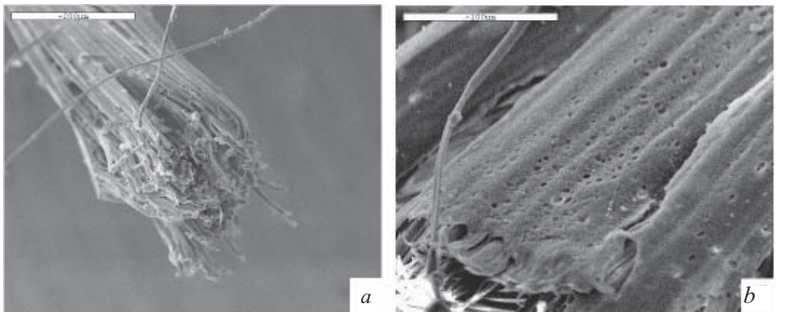

Fig. 2. Electron-microscopic photograph of samples of Ftorlon fibres: *a*) initial fibre; *b*) Ftorlon + polymer.

regression equation poly(*x,y*), presented below, and construction of the three-dimensional polynomials were the result of running the software.

$$\text{coeff}\, s = \begin{pmatrix} 0 \\ 2.936 \cdot 10^{-3} \\ -0.026 \\ 16.703 \\ -0.865 \\ 0.294 \end{pmatrix} \quad I = \begin{pmatrix} 1 & 1 \\ 0 & 2 \\ 0 & 1 \\ 0 & 0 \\ 1 & 0 \\ 2 & 0 \end{pmatrix}$$

$$\text{poly}(x,y) := \sum_{i=0}^{\text{last}(\text{coeff}\, s)} \left(\text{coeff}\, s_i \cdot x^{I_{i,0}} y^{I_{i,1}} \right)$$

This equation describes the results of the experiment on determination of the linear density. When the numerical values of the modification parameters are substituted in it, the results of the calculations maximally approach the experimental data. The regression equation more graphically describes the results of the experiment by constructing the polynomial of the effect of the modification conditions on the output parameter.

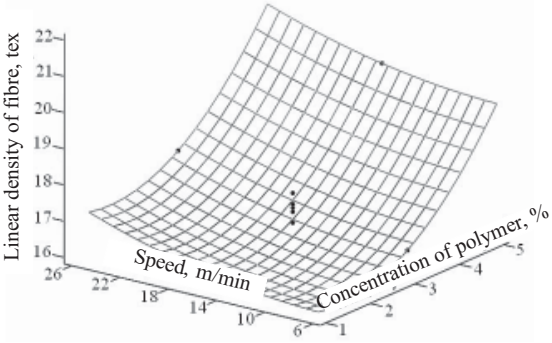

Fig.3

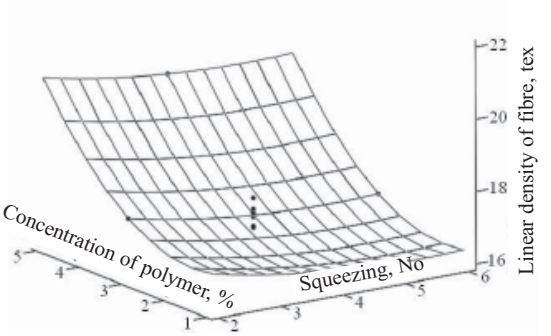

Fig.4

Fig. 3. Polynomial of the linear density of Ftorlon bicomponent fibre as a function of the concentration of polymer in the modifying solution and rate of fibre movement for 4 squeezing rings.

Fig. 4. Polynomial of the linear density of Ftorlon bicomponent fibre as a function of the number of squeezed sections and concentration of polymer in the modifying solution at a takeup rate of 15.5 m/min.

TABLE 3. Dependence of the Strength of the Bicomponent Fibre on the Modifying Polymer Content

Concentration of the solution, %	Ftorlon fibre			PCA fibre		
	ω, %	*h*, μm	P_b, cN	ω, %	*h*, μm	P_b, cN
Initial fibre	0	0	528	0	0	1027
1.0	0.8±0.1	0.2	619±1	0.5±0.1	0.2	1147±2
1.8	1.0±0.2	0.4±0.1	647±2	2±1	1.0±0.2	1166±2
3.0	6.0±1.5	1.5±0.5	666±3	10±2	4.5±0.5	1178±4
4.2	10±2	3.0±0.5	717±2	16.5±1.5	8±0.5	1180±3
5.0	19±2	6.0±0.5	738±4	21±2	10±1	1190±4

Notation: ω — modifying polymer content in bicomponent fibre; *h*— thickness of modifying layer; P_b — breaking load.

These mechanisms of the effect of the process parameters of application of coatings on the properties of the modified bicomponent fibres were characterized in the form of three-dimensional dependences of the optimization parameter on two variable application parameters constructed with the calculated regression equation.

The data in Figs. 3 and 4 show that the linear density of the modified Ftorlon fibre increases with an increase in the concentration of the modifying solution, fibre takeup rate, and a decrease in the number of squeezing rings. The last two parameters have a weak effect. Note that only the lower three squeezing rings effectively remove excess solution from the fibre while the 4th, 5th, and 6th rings do not affect the linear density, probably due to drying of the modifying solution and difficult removal of the excess. The increase in the linear density when the rate increases is due to a decrease in the duration of interaction of the squeezing rings with the modified fibre, which reduces the amount of modifying solution removed. The interdependence in modification of PCA fibre seems similar, but no effect of the degree of squeezing is not observed at all in this case (Fig. 5).

Application of a coating on the fibre causes a greater increase in the breaking load the thicker the layer of the modifying coating (Table 3), which is due to an increase in the interfibre cohesive force.

Modification also increases the breaking load P_0, expressed in cN/tex, but it follows from the data in Figs. 6 and 7 that P_0 is inversely dependent on the content of modifying polymer on the fibre. Note also that P_0 decreases with an increase in the fibre takeup rate and is not a function of the degree of squeezing. These dependences are due to the increase in the linear density of the fibre (Figs. 3-5) and application of the unoriented and correspondingly less strong layer.

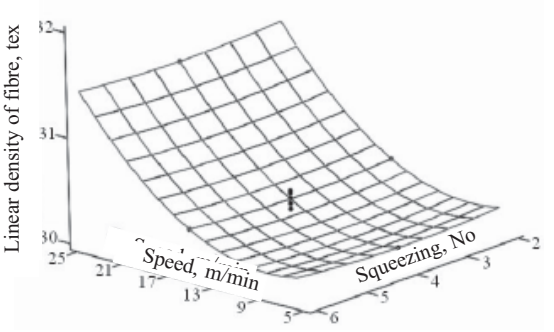

Fig.4

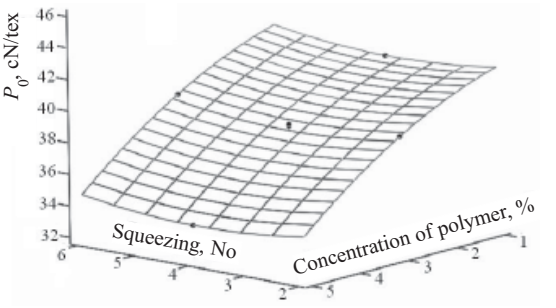

Fig.5

Fig. 5. Polynomial of the linear density of PCA bicomponent fibre as a function of the fibre movement rate and number of squeezed sections at a 3% concentration of the modifying solution.

Fig. 6. Polynomial of the strength of PCA bicomponent fibre as a function of the amount of squeezed sections and concentration of polymer in the modifying solution at a fibre speed of 15.5 m/min.

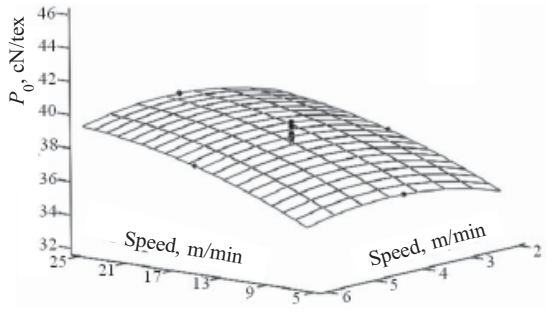

Fig.6

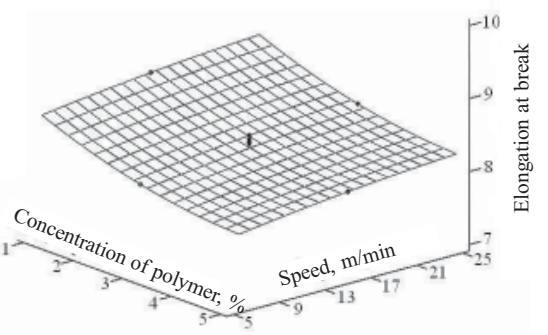

Fig.7

Fig. 7. Polynomial of the strength of Ftorlon bicomponent fibre as a function of fibre speed and number of squeezed sections at a 3% concentration of modifying solution.

Fig. 8. Polynomial of the elongation at break of bicomponent Ftorlon fibre as a function of the concentration of polymer in the modifying solution and fibre speed for 4 squeezing rings.

Figure 8 shows that the concentration of the solution and the takeup rate weakly affect the elongation at break of the bicomponent fibre, i.e., the elastic properties, almost do not change. The tendency toward a decrease in the elongation at break with an increase in the concentration of the polymer and consequently the amount of applied modifier can be explained by formation of a pseudomonofilament, high adhesion of the filaments in the core—shell structure and consequently, and their simultaneous breaking in deformation.

It is important to note that the mathematical models in the form of regression equations and polynomial curves give reliable results of calculations of the optimization parameters only on substitution of the initial parameters which do not go beyond the limits of the numerical values of the conditions of the modeled experiment. The equations obtained and their graphic image can be used for analyzing the experiment and looking for the optimum values only for interpolation, but not for extrapolation.

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