Mathematical Modeling Of Rheological Behavior Of Anisotropic Biomaterials With Taking Into Account Effects Of Memory And Self-organization

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Abstract

Research and prediction of the physical properties of biomaterials and biostructures are associated with the effects of memory, spatial correlation and self-organization processes. Taking into account the fractal structure of biomaterials allows us to identify new regularities of their behavior in mechanical and related processes. Mathematical models of non-isothermal moisture transfer and visco-elastic deformation in biomaterials with taking into account the fractal structure of the environment was constructed. One-dimensional mathematical models of deformation-relaxation processes in environments with fractal structure which characterized by the effects of memory, spatial nonlocality and self-organization are considered. Taking into account that the fractional parameters of fractal models allow to describe the deformation-relaxation processes in biomaterials in comparison with traditional methods more fully in the paper, the optimal approximation method, the Proni's method was proposed. This method allows to reduce the problem of identification the fractional parameters which are the part of the creep and relaxation kernels structure to finding the solutions of systems of linear equations. Software to implement the obtained models was developed.

Keywords 1

Moisture transfer, visco-elastic deformation, effects of memory, Proni's method, finite-difference method

1. Introduction

Investigation of deformation-relaxation processes have shown that the using of fractional integrate-differential apparatus for modeling those processes allows more appropriately, on the basis of physical considerations, generalize experimental data to identify model parameters [1, 3, 5]. Particularly important are the works devoted to research of regular and irregular modes of the process of heat treatment of biomaterials in terms which makes it possible to take into account the effects of "memory" and self-organization of the material. Initially, there are studies to find an effective method for identifying fractal parameters of models [2, 4, 5].

Replacing real environment properties with their idealized models is based on the fact that the some of the properties of this environment appear most clearly. Then, by rejecting everything that is irrelevant, the ideal model can be constructed which be characterized by these dominant

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characteristics of real environment. In particular, considering only the properties of elasticity and viscosity, it is possible to construct the simpler rheological models that are used in viscosity theory studies. They can be formed by the series or parallel connection of the elastic element, behavior of which obeys to the Hooke's law, and the viscous, obeys to the Newton's law of viscosity [14, 22].

The simpler models which are constructed by that way will not take into account material properties such as "memory", the complex nature of spatial correlations, and the self-organizing effects that are characterize for biomaterial [9, 11]. Therefore, it is suggested to use the fractional-order integro-differentiation mathematical apparatus to record the Newton's law of viscosity, which will allow take into account the above mentioned properties of this material [6-8, 10, 12, 13].

This work is devoted to solving the actual scientific task of increasing the efficiency of mathematical modeling of heat and mass transfer processes and visco-elastic deformation of biomaterials with taking into account the effect of "memory" and self-organization in the heat treatment process to provide appropriate quality of the material.

The algorithm of identification of fractal parameters of models was developed, which is based on the use of the iterative method and co-ordinate descent. The experimental data of biomaterial creep was approximated using fractional exponential operators also identified relationship between the fractional component and materials species, temperature and humidity fields.

The characteristics of the heat and moisture transfer processes and stress-strain state during heat treatment process with accounting the fractal structure of material with different thermo-mechanical material parameters treatment modes were analyzed.

2. Production of a problem

2.1. The visco-elastic deformation problem

The mathematical model of the rheological behavior of anisotropic capillary-porous materials in the heat treatment process with taking into account the fractal structure of the environment can be described by equations of equilibrium with fractional order γ $(0<\gamma\le 1)$ in spatial coordinates x_1 and x_2 for the sample with such spatial dimensions $\Omega=\{x_1;x_2\}=\{[0;l_1]\times[0;l_2]\}$ [15, 16, 18, 19]:

$$C_{11}\left(\frac{\partial^\gamma\varepsilon_{11}}{\partial x_1^\gamma}\left(1-\overline{R}_{11}\right)-\frac{\partial^\gamma\varepsilon_{T1}}{\partial x_1^\gamma}+\widetilde{R}_{11}\right)+C_{12}\left(\frac{\partial^\gamma\varepsilon_{22}}{\partial x_1^\gamma}\left(1-\overline{R}_{12}\right)-\frac{\partial^\gamma\varepsilon_{T2}}{\partial x_1^\gamma}+\widetilde{R}_{12}\right)+ \\ +2C_{33}\left(\frac{\partial^\gamma\varepsilon_{12}}{\partial x_2^\gamma}\left(1-\overline{R}_{33}^2\right)-\frac{\partial^\gamma\varepsilon_{T3}}{\partial x_2^\gamma}+\widetilde{R}_{33}^2\right)=0, \tag{1}$$

$$C_{21}\left(\frac{\partial^\gamma\varepsilon_{11}}{\partial x_2^\gamma}\left(1-\overline{R}_{21}\right)-\frac{\partial^\gamma\varepsilon_{T1}}{\partial x_2^\gamma}+\widetilde{R}_{21}\right)+C_{22}\left(\frac{\partial^\gamma\varepsilon_{22}}{\partial x_2^\gamma}\left(1-\overline{R}_{22}\right)-\frac{\partial^\gamma\varepsilon_{T2}}{\partial x_2^\gamma}+\widetilde{R}_{22}\right)+ \\ +2C_{33}\left(\frac{\partial^\gamma\varepsilon_{12}}{\partial x_1^\gamma}\left(1-\overline{R}_{33}^1\right)-\frac{\partial^\gamma\varepsilon_{T3}}{\partial x_1^\gamma}+\widetilde{R}_{33}^1\right)=0 \tag{2}$$

Where $\varepsilon^T=(\varepsilon_{11},\varepsilon_{22},\varepsilon_{12})$, $\varepsilon_T=(\varepsilon_{T1},\varepsilon_{T2},\varepsilon_{T3})^T$ – deformation vectors, vector components ε_T caused by changes in temperature ΔT and moisture content ΔU:

$$\begin{aligned}\varepsilon_{T1}&=\alpha_{11}\Delta T+\beta_{11}\Delta U,\\ \varepsilon_{T2}&=\alpha_{22}\Delta T+\beta_{22}\Delta U,\\ \varepsilon_{T3}&=0.\end{aligned} \tag{3}$$

where $\alpha_{11},\alpha_{22},\beta_{11},\beta_{22}$ – coefficients of temperature expansion and humidity compression; C_{ij} – components of the elasticity tensor of the orthotropic body, $\overline{R}_{ij}$, $\widetilde{R}_{ij}$ – value of integrals of relaxation kernels of fractional-differential models:

$$\int_0^t R_{ij}(t-z,T,U)dz = \overline{R}_{ij},$$
$$\int_0^t R_{ij}(t-z,T,U)\frac{\partial^\gamma \varepsilon_{T1,T2}}{\partial x_k^\gamma}dz = \widetilde{R}_{ij}, \tag{4}$$
$$\int_0^t R_{ij}(t-z,T,U)\frac{\partial^\gamma \varepsilon_{T3}}{\partial x_2^\gamma}dz = \widetilde{R}_{33}^2$$

We set the following boundary and initial conditions:

$$\varepsilon_{ij}\big|_{x_j=0} = 0,$$
$$\varepsilon_{ij}\big|_{x_j=l_j} = 0, \tag{5}$$
$$\varepsilon_{ij}\big|_{t=0} = 0, \ (j=1,2)$$

Also the stress-deformable state of biomaterial components should be satisfies the equation of equilibrium.

2.2. The heat-mass transfer problem

The mathematical model of the distribution of temperature-humidity fields in biomaterials with a fractal structure, the stress-strain state of which is discussed in the paragraph 2.1, is described by a system of differential equations in partial derivatives of fractional order by time τ and spatial coordinates x_1 and x_2 [7, 8, 13, 17, 18, 20, 21]:

$$c\rho\frac{\partial^\alpha T}{\partial \tau^\alpha} = \lambda_1\frac{\partial^2 T}{\partial x_1^2} + \lambda_2\frac{\partial^2 T}{\partial x_2^2} + \varepsilon\rho_0 r\frac{\partial^\alpha U}{\partial \tau^\alpha};$$
$$\frac{\partial^\alpha U}{\partial \tau^\alpha} = a_1\frac{\partial^2 U}{\partial x_1^2} + a_2\frac{\partial^2 U}{\partial x_2^2} + a_1\delta\frac{\partial^2 T}{\partial x_1^2} + a_2\delta\frac{\partial^2 T}{\partial x_2^2}. \tag{6}$$

and appropriate initial conditions

$$T(\tau,x_1,x_2)\big|_{\tau=0} = T_0(x_1,x_2);$$
$$U(\tau,x_1,x_2)\big|_{\tau=0} = U_0(x_1,x_2). \tag{7}$$

and boundary conditions of third kind

$$\begin{cases} \lambda_i\dfrac{\partial T}{\partial n}\Big|_{x_i=l_i} + \rho_0(1-\varepsilon)\beta\left(U\big|_{x_i=l_i} - U_P\right) = \alpha_i(T\big|_{x_i=l_i} - t_c) \\ a_i\delta\dfrac{\partial T}{\partial n}\Big|_{x_i=l_i} + a_i\dfrac{\partial U}{\partial n}\Big|_{x_i=l_i} = \beta\left(U_P - U_{x_i=l_i}\right) \end{cases} \tag{8}$$

$$\begin{cases} \lambda_i\dfrac{\partial T}{\partial n}\Big|_{x_i=0} + \rho_0(1-\varepsilon)\beta\left(U\big|_{x_i=0} - U_P\right) = 0 \\ a_i\delta\dfrac{\partial T}{\partial n}\Big|_{x_i=0} + a_i\dfrac{\partial U}{\partial n}\Big|_{x_i=0} = 0 \end{cases} \tag{9}$$

where, $T(\tau,x_1,x_2)$ - temperature, $U(\tau,x_1,x_2)$ - humidity, $c(T,U)$ - thermal capacity, $\rho(U)$ - density, ρ_0 - basis density, ε - phase transition coefficient, r - heat of vaporization, $\lambda_i(T,U)$ - coefficients of thermal conductivity, $a_i(T,U)$ - coefficients of humidity conductivity, $\delta(T,U)$ - thermogradient coefficient, t_c - ambient temperature, U_p - relative humidity of the environment, $\alpha_i(t_c,v)$ - heat transfer coefficient, $\beta(t_c, \varphi, \nu)$ - moisture transfer coefficient, α - fractional order of derivative by the time $(0 < \alpha \le 1)$.

3. Identification of fractional-exponential creep kernels by approximation the experimental data using the Proni's method

The mathematical model (1)-(2) of visco-elastic deformation in fractal media for the one-dimension case can be written using the Boltzmann-Volterr's integral equation [16]:

$$\varepsilon(t) = \sigma_0 G(t) + \int_0^t \Pi(t - z, T, U) D_z^{\alpha} \sigma(z) dz \tag{10}$$

$$\sigma(t) = \varepsilon_0 G'(t) + \int_0^t R(t - z, T, U) D_z^{\beta} \varepsilon(z) dz \tag{11}$$

where t - time; $\alpha = \alpha(T,U), \beta = \beta(T,U)$ - fractional order of the derivative which are dependent on temperature T and moisture U; $\varepsilon(t)$ - deformation; $\sigma(t)$ - tension; ε_0, σ_0 - the value of deformation and tension on the initial time moment t_0; $G(t), G'(t)$ - time dependent functions; $\Pi(t - z, T, U)$, $R(t - z, T, U)$ - creep and relaxation kernels (memory functions), D_z^{α}, D_z^{β} – fractional derivatives by the variable z with the order α, β $(0 \le \alpha, \beta \le 1)$ accordingly.

The general view of the creep kernel for fractional-differential rheological models (1)-(5) will be follows [16]:

$$\Pi(t) = \frac{1}{E\tau^{\beta}} t^{\beta - 1} E_{\psi_1, \psi_2}(\varphi) \tag{12}$$

where E- modulus of elasticity, $\tau = \eta / E$ (η - the coefficient of viscosity), $E_{\psi_1,\psi_2}(\varphi)$ - the Mittag-Leffler's function, $(\psi_1 = \psi_1(\alpha, \beta), \psi_2 = \psi_2(\alpha, \beta), \varphi = \varphi(t, \alpha, \beta))$.

Since the Proni's approximation method, which is valid for a linear combination of exponential functions, will be used to parameters identification of creep data the equation (11) will be transformed in the paper.

The two-parameter Mittag-Leffler function is given by the formula [16]:

$$E_{\alpha,\beta}(t) = \sum_{j=0}^{\infty} \frac{t^j}{\Gamma(\alpha j + \beta)} \tag{13}$$

Taking into account the equation (12) and the corresponding substitutions, we rewrite the appearance of the creep kernel (11) as follows:

$$\Pi(s) = \sum_{i=0}^{n} A_i e^{-\lambda_i s} \tag{14}$$

where $A_i = A_i(\alpha, \beta)$, $\lambda_i = \lambda_i(\alpha, \beta)$ - amplitudes and indices dependent on the fractional parameters α, β, $s = \ln t$, $(t = e^s)$.

In [16] it is pointed out that for functions which have the form such as $\Pi(s)$ there is some definite linear relationship between its $(n+1)$ equidistant values:

$$\sum_{i=0}^{n} c_i \Pi(s + ih) = 0 \tag{15}$$

where c_i - searching constant values $(c_n = 1)$, h- the time interval is longer than between two consecutive values.

Since (13) is a solution of equation (14), then parameters λ_i can be found by using this method.

Let $e^{-\lambda_i h} = \xi_i$ then to determine each value ξ_i we need to solve the algebraic equation:

$$c_0 + \sum_{i=1}^{n} c_i \xi^i = 0 \tag{16}$$

To determine c_i the following system of linear equations must be solved:

$$\begin{cases} \Pi_1^* c_0 + \Pi_2^* c_1 + \ldots + \Pi_n^* c_{n-1} + \Pi_{n+1}^* = 0, \\ \Pi_2^* c_0 + \Pi_3^* c_1 + \ldots + \Pi_{n+1}^* c_{n-1} + \Pi_{n+2}^* = 0, \\ \ldots \\ \Pi_n^* c_0 + \Pi_{n+1}^* c_1 + \ldots + \Pi_{2n-1}^* c_{n-1} + \Pi_{2n}^* = 0, \end{cases} \tag{17}$$

where $\Pi_1^*, \Pi_2^*, \ldots, \Pi_{2n}^*$ - ordinates.

Finding from (15) the n solutions $\xi = \xi_1, \xi_2, \ldots, \xi_n$ we can find the parameters λ_i:

$$\lambda_i = -\frac{\ln \xi_i}{h} \tag{18}$$

To determine the amplitudes A_i you must determine the n ordinates - $\Pi_1^*, \Pi_2^*, \ldots, \Pi_n^*$ and also find the solution of the following system of linear equations:

$$\begin{cases} A_1' + A_2' + \ldots + A_m' = \Pi_1^*, \\ A_1' p_1 + A_2' p_2 + \ldots + A_m' p_m = \Pi_2^*, \\ \ldots \\ A_1' p_1^{n-1} + A_2' p_2^{n-1} + \ldots + A_m' p_n^{n-1} = \Pi_n^*, \end{cases} \tag{19}$$

where $p_i = e^{-\lambda_i h}$, $A_i' = \dfrac{A_i e^{-\lambda_i s_0}}{\lambda_i}$, $\left(i = \overline{1, n}\right)$, s_0 - initial time moment.

The fractionally-exponential creep kernels can be identified according to the following experimental data [20], which are given in Table 1.

Table 1
Experimental creep data

k	Π_k (mm)	k	Π_k (mm)	k	Π_k (mm)	k	Π_k (mm)
1	2,2	7	2,82	13	2,93	19	0,88
2	2,31	8	2,85	14	2,94	20	0,86
3	2,61	9	2,87	15	1	21	0,84
4	2,68	10	2,9	16	0,9	22	0,79
5	2,73	11	2,91	17	0,85	23	0,77
6	2,75	12	2,93	18	0,87	24	0,74

To determine the fractional parameters α and β it is suffices for each rheological model to distinguish two exponential functions, that is we consider the relation (13) for the case $n = 2$. Accordingly, the 2^n ordinates are required to find λ_i parameters. To do this, let's break down the experimental data into 4 groups by summing up six ordinates in each. As a result of calculations we get that $\Pi_1^* = 15{,}28$; $\Pi_2^* = 17{,}28$; $\Pi_3^* = 9{,}49$; $\Pi_4^* = 4{,}88$. The system of linear equations (16) will look like:

$$\begin{cases} 15{,}28 c_0 + 17{,}28 c_1 + 9{,}49 = 0, \\ 17{,}28 c_0 + 9{,}49 c_1 + 4{,}88 = 0. \end{cases} \tag{20}$$

Wherefrom $c_0 = 0{,}0373$, $c_1 = -0{,}5822$. The algebraic equation (15) will have the form:

$$\xi^2 - 0.5822\xi + 0{,}0373 = 0. \tag{21}$$

The roots of which are equal respectively $\xi_1 = 0{,}5089$, $\xi_2 = 0{,}0733$.

The initial time moment according to our experimental data is $t_0 = 10^3$ (h) and step $\Delta t = 500$ (h). Taking into account the corresponding replacement of variables, the h value in formula (17) will be equal to 37,2876.

The values of λ_i will be follows: $\lambda_1 = 0{,}0181$, $\lambda_2 = 0{,}0701$.

Here are obtained creep kernels for the Maxwell's, Voigt's and Kelvin's fractional-differential models:

$$\Pi_M(t) = \frac{1}{E\tau^\beta}\left(\frac{t^{\beta-1}}{\Gamma(\beta)} + \frac{\tau^\alpha t^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}\right),\ 0 \le \alpha < \beta \le 1 \qquad (22)$$

$$\Pi_F(t) = \frac{1}{E\tau^\beta} t^{\beta-1} E_{\beta-\alpha,\beta}\left(-\frac{t^{\beta-\alpha}}{\tau^{\beta-\alpha}}\right),\ 0 \le \alpha < \beta \le 1 \qquad (23)$$

$$\Pi_K(t) = \frac{t^{\beta-1}}{E\tau^\beta} E_{\beta,\beta}\left(-\frac{t^{\beta-\alpha}}{\tau^{\beta-\alpha}}\right),\ 0 \le \alpha \le 1, 0 < \beta \le 1 \qquad (24)$$

Accordingly, for the Maxwell's model the parameters will be determined from the ratios: $\lambda_1 = 1-\beta$, $\lambda_2 = 1+\alpha-\beta$. From where we find that the fractional-differential parameters are: $\alpha = 0{,}0520$, $\beta = 0{,}9819$.

Using formula (12) we find parameters λ_1 and λ_2 for the Voigt and Kelvin models, which will have the following view: $\lambda_1 = 1+\alpha-2\beta$, $\lambda_2 = 1-\beta$. The fractional-differential parameters will have the following values: $\alpha = 0{,}8779$, $\beta = 0{,}9299$.

The parameters α and β which describe the creep kernel are functionally dependent on the humidity and temperature of the medium. The experimental creep data were investigated at temperature $T = 23°C$, humidity $U = 65\%$ and elastic modulus $E = 13800 \text{МП}a$.

In the expressions which describe the creep kernels, the parameter τ $\left(\tau = \eta/E\right)$ where η - viscosity is still unknown. We find it by finding the amplitudes A_i. To do this, we must solve the system of linear equations (18):

$$\begin{cases} A_1' + A_2' = 15{,}28; \\ A_1' p_1 + A_2' p_2 = 9{,}49; \end{cases} \qquad (25)$$

where $p_1 = e^{-0{,}6749}$, $p_2 = e^{-2{,}6139}$.

Having found $A_1' = 19{,}2008$ and $A_2' = -3{,}9208$, when $s_0 = 6{,}9078$ we obtain the following values of amplitudes: $A_1 = 0{,}3938$, $A_2 = -0{,}4460$.

Since A_2 it is not in the range of amplitude values, we find the τ parameter value from A_1, $\left(A_1 = \tau^{-\beta}/E\Gamma(\beta)\right)$. For Maxwell and Voigt models the parameter $\tau_{M,F} = 0{,}155 \cdot 10^{-3}$, for Kelvin is $\tau_K = 0{,}975 \cdot 10^{-2}$.

4. Obtained results

4.1. The parameter identification result

For the sample of biomaterial, whose modulus of elasticity is $(\mathrm{E} = 13{,}8 МПa)$ with the humidity value $(W = 45\%)$, the fractional-differential parameters identification were conducted for the Maxwell, Kelvin and Voigt models by the Proni's method.

The deformation curves (12) identified from the experimental biomaterial creep data [21] for the Voigt model (Fig. 1), as well as for the Maxwell and Kelvin models. They were investigated under constant load and in the absence thereof.

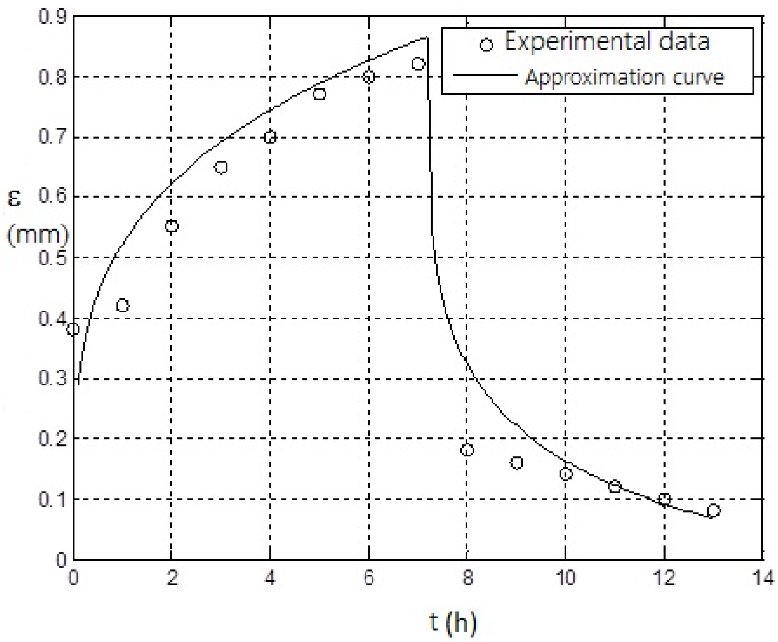

Figure 1: Identification of fractional-differential parameters for the Voigt model at biomaterial humidity W=15%

The obtained graphical dependences of deformations depending on time are similar to the well-known model of hygro(thermo)-mechanical deformations which describe the deformations in biomaterial with change of its load, temperature and humidity. The developed model also takes into account the formation of residual deformations which are characterized by the "memory" effects of biomaterial. According to Fig. 1 after unloading of the material the creep deformities remain. The maximum deviation of the approximate values from the experimental values does not exceed 4,7%. It can be concluded that an approximant in the form of a linear combination of Mittag-Leffler's functions is an effective tool for approximation the experimental creep data of biomaterial.

Thus, the experimental data of biomaterial creep were approximated using fractional-exponential functions and their fractional parameter was distinguished which are characterizing the influence of the fractal structure of the material. The coefficients of creep and relaxation kernels which are necessary for implementation the mathematical model of heat-mass transfer (6)-(9) and viscoelastic deformation (1)-(5) of biomaterials with fractal structure are obtained.

4.2. The visco-elastic deformation result

Let's carry out a numerical implementation of the mathematical model (1)-(5) of visco-elastic deformation using the fractional-Voigt model as a basis. Considering the results of identification we will select the following values of parameters: E = 5,19 (GPa), W = 45%, fractional order of the model - $\alpha = 0{,}8856$. The finite-difference method described in [10, 16, 19] is used to find the numerical solution of the two-dimensional visco-elastic deformation problem. The dynamics of the stress components σ_{12} for different biomaterial species depending on change of fractal items is shown as an example.

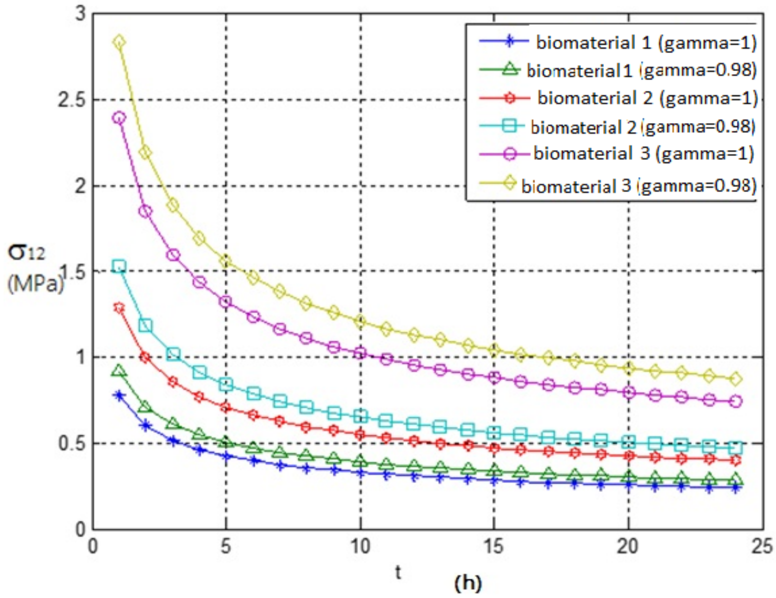

Figure 2: Dynamics of the stress components σ_{12}

The influence of fractal parameters on the dynamics of stresses and strains components depending on time is analyzed (Fig. 2). It is established that the difference between the stress components with taking into account the fractal structure and without for biomaterial with higher density does not exceed 16.7%, but the difference for the biomaterial with lower density reaches 19.6 - 24%.

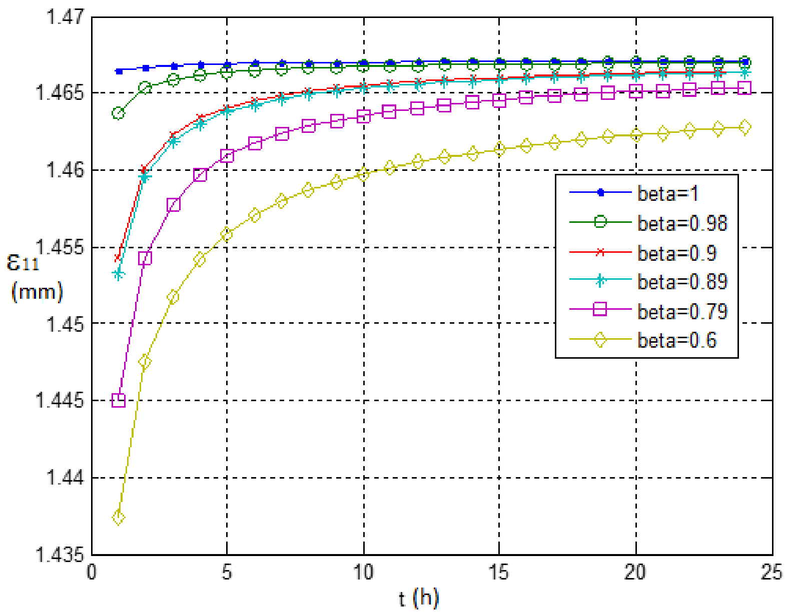

Figure 3: Dynamics of the deformation components ε_{11}

In Fig. 3 and Fig. 4 the dynamics of the deformation components ε_{11}, ε_{22} for the biomaterial depending on the change of the fractal element β is investigated. The remaining fractal parameters did not change in the process of numerical implementation and took the following values - $\alpha = 0.5$, $\beta = 0.5$.

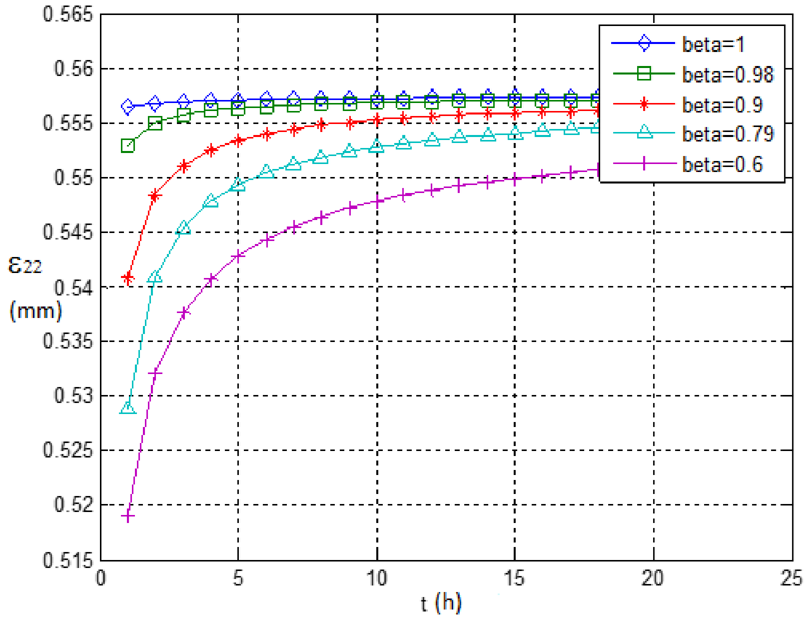

Figure 4: Dynamics of the deformation components ε_{22}

The deformation curves for the integer parameter $\beta = 1$ differ significantly from the curves using the fractal parameter β. The deformations in the radial direction of the anisotropy of biomaterials with taking into account the fractal structure are greater than in the tangential.

5. Conclusion

Taking into account the two-parameter Mittag-Leffler function and the corresponding substitutions the general appearance of the original problem is reduced to the standard form of a linear combination of exponential functions which makes it possible to use the Proni's method. Fractional-differential parameters for mathematical models of Maxwell, Kelvin, and Voigt viscous-elastic deformation in biomaterials by experimental creep kernels curves are identified. The properties of fractional order for each mathematical model of visco-elastic deformation in fractal media are taken into account and analyzed on parameters approximating process. And the other conditions that must be fulfilled for applying the Proni's method described above.

The obtained results can be used for further investigation of mathematical models of visco-elastic deformation processes in biomaterials, as in media with a fractal structure.

For the fractional Voigt model for biomaterial with high density the identification method (iterative method) was chosen correctly, since the approximated curves are in good agreement with the experimental data. During the study of the creep of the biomaterial during, it is possible to record the formation of residual deformations, the magnitude of which is defined as the difference between the visco-elastic deformations in the initial state (heated or wet biomaterial) and the end state (chilled or dry biomaterial). Residual stresses describe the memory effect of biomaterial . Developed methods and algorithms of parametric identification of rheological models of creep and relaxation for the study of viscoelastic behavior of biomaterials by using experimental data allow to calculate the parameters of the models, in particular the orders of fractional derivatives. Numerical studies have shown that the described algorithms and techniques are characterized by sufficient efficiency. They can be used to solve problems of parametric identification of generalized rheological models with using fractional derivatives.

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