Variational Formulation Of Viscoelastic Problem In Biomaterials With Fractal Structure

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Abstract

A mathematical model of the viscoelastic deformation problem for biomaterials with fractal structure is constructed. The basic relationships between stress-strain state components of the rheological behavior of the biomaterials during heat treatment are obtained. Integro-differentiation apparatus of fractional order to account the fractal structure of the considering biomaterial was used. The fractal integral relations for determining the components of the stress vector due to deformation were obtained. A variational formulation of the viscoelastic deformation problem of biomaterials with taking into account their fractal structure is obtained. Which allows to obtain an approximate continuous solution of the problem. Application software for finding an approximate solution of the viscoelastic deformation problem of biomaterials with taking into account their fractal structure was developed. The usecase diagram of the developed software and the sequence diagram for usecase which provides reception of a numerical decision were constructed. For partial cases the numerical solutions of this problems was obtained are analyzed. The dependence of stress components on the degree of material fractality, geometric sizes and type of biomaterials were analyzed.

Keywords [1]

Fractal structure, stress, strain, variation formulation, finite element method

1. Introduction

The development of additive technologies based on the active use of mathematical and computer modeling and introduction of special innovative information technologies in medicine, the permanent expansion of the range of bioprosthetics applications, appearance of materials with new properties and capabilities led to an integrated interaction of mechanics, computer science and medicine. The construction of mechanical and mathematical models for describing the state and behavior of biomaterials and biostructures, the studying of their physical and mechanical properties is an important area of research [2, 4, 6, 14].

The study of the patterns of displacement and deformation of biological structures and tissues under the influence of external environment factors and the muscular system is an urgent scientific task. It is connected with the facts that in the process of evolution biological systems have arisen that are optimal in design with not only regard to the physiological functions they perform, but also the properties of materials which determining their mechanical behavior. Therefore, the study of the structure and mechanical properties of various biological tissues will make it possible to create materials most suitable for replacing damaged natural structures [8].

Knowledge of the quantitative and qualitative indicators of the state and dynamics of the biomaterials properties allows to obtain new information about their functioning and vital activity and provides data to improve the accuracy of diagnosis and improve the quality of therapy for various diseases. Therefore, the construction of mechanical and mathematical models for studying the

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behavior of biomaterials based on the fractional order integro-differentiation apparatus, the development of highly effective analytical and experimental methods for assessing the physical and mechanical properties of biomaterials is an urgent scientific task [5, 10, 11, 13, 24].

A significant number of real processes do not fit into the concepts of continuum mechanics and requires to use the involvement of ideas about the fractality of the environment in which these processes occur. The viscoelastic deformation of biomaterials refers to such processes. The correspondingly modified relations of the theory of viscoelasticity are used to describe them, which requires the use of the mathematical apparatus of fractional integro-differential calculus. Yu.N. Rabotnov introduced a generalization of the rheological equation to describe the behavior of hereditary media using the apparatus of fractional derivatives [19-23, 25].

Taking into account the effect of memory by fractional derivatives in mathematical models leads to an increasing in computational costs when finding a numerical solution. Any algorithm that uses the sampling of fractional order derivatives must take into account its nonlocality, which leads to increasing storage requirements for computational data and the complexity of the algorithm. Numerical algorithms for finding the solution of differential and integral equations containing fractional order operators can be found in the literature devoted to so-called collocation methods for solving Voltaire-Abel integral equations. There are also works devoted to the consideration of fractional-linear multi-step methods for the numerical solution of such integral equations [3, 7, 9, 15, 16, 31].

One of the problems that arise when using fractional derivatives is that there is no unambiguous definition of them. Numerical methods for solving problems which describes by equations with fractional derivatives are tied to the type of the chosen derivative, so there is a need to analyze and compare the results obtained using different definitions and numerical methods.

Thus, the construction of the variational formulation of the viscoelastic deformation problem of biomaterials with taking into account their fractal structure is an urgent scientific problem. Its solution will make it possible to obtain the values of the stresses, strains and displacements components as continuous functions. Analyzing the obtained values, we can conclude about the strength and rheological behavior of biomaterials, which is an important characteristic in their operation.

2. Production of a problem

Integrals and derivatives of fractal order and fractional integro-differential equations find many applications in modern research in theoretical physics, mechanics and applied mathematics. Fractional mathematical calculus is a powerful tool for describing physical systems that have memory and nonlocality effects [26, 28]. Using of fractional mathematical analysis can be useful for obtaining dynamic models in which integro-differential operators by the time and spatial coordinates describe the degree of long-term memory and spatial nonlocal complex structure of environments and processes. Let us consider the fractional order integro-differentiation operators integral of the function $f(x,y,z)$ over the variable x in Caputo's understanding in more detail [12, 18, 32-34].

$$D_x^\alpha f = \frac{1}{\Gamma(1-\{\alpha\})}\int_a^x \frac{\partial^{[\alpha]+1} f(\xi,y,z)}{\partial \xi^{[\alpha]+1}}\frac{d\xi}{(x-\xi)^{\{\alpha\}}}, \tag{1}$$

$$I_x^\alpha f = \frac{1}{\Gamma(\{\alpha\})}\int_a^x \frac{\partial^{1-[\alpha]} f(\xi,y,z)}{\partial \xi^{1-[\alpha]}}\frac{d\xi}{(x-\xi)^{\{\alpha\}}}, \tag{2}$$

where $\alpha = [\alpha]+\{\alpha\},\ [\alpha]\in N,\ 0<\alpha<1,\ \Gamma(\alpha)=\int_0^\infty x^{\alpha-1}e^{-x}dx$ - gamma function.

2.1. The viscoelastic deformation problem

Let’s consider the problem of stress-strain state in biomaterial with taking into account the fractal structure. Suppose that a body which is in equilibrium is affected by mass forces $\overline{\mathbf{F}} = \left(\rho\overline{X}, \rho\overline{Y}, \rho\overline{Z}\right)^T$ in the corresponding directions. And also surface forces $\overline{\mathbf{F}}_V = \left(\overline{X}_V, \overline{Y}_V, \overline{Z}_V\right)^T$ with corresponding projections on the axis x, y, z. Let's find the components of the stress-strain state of the body, namely vectors $\boldsymbol{\sigma} = \left(\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{xz}, \tau_{yz}\right)^T$ - stress, $\boldsymbol{\varepsilon} = \left(\varepsilon_x, \varepsilon_y, \varepsilon_z, \gamma_{xy}, \gamma_{xz}, \gamma_{yz}\right)^T$ - deformation and displacement $\mathbf{u} = (u, \upsilon, \omega)^T$, which are satisfying the equilibrium equation in elementary volume [27, 29, 30]

$$D_{x_j}^{\alpha} \sigma_{ij} + \overline{F_i} = 0, \tag{1}$$

and the equilibrium conditions on the surface [17]

$$\overline{F}_{V\,i} = \sigma_{ij} \cos(n, x_j), \tag{2}$$

where n- outer normal to the surface of the body S.

The relationship between displacements and deformations will be written with using the derivatives of fractal order as follows [29, 30]

$$\varepsilon_{ij} = \frac{1}{2}\left(D_{x_j}^{\alpha} \mathbf{u}_i + D_{x_i}^{\alpha} \mathbf{u}_j\right). \tag{3}$$

Thus, the relations between stress and deformation components with using the integral of fractal order are written as follows [30]:

$$\sigma_x = \varepsilon_x - I_t^{\alpha}\left[R_{11}(t - \tau_{rel})\varepsilon_x\right] + \varepsilon_y - I_t^{\alpha}\left[R_{12}(t - \tau_{rel})\varepsilon_y\right] + \varepsilon_z - I_t^{\alpha}\left[R_{13}(t - \tau_{rel})\varepsilon_z\right], \tag{4}$$

$$\sigma_y = \varepsilon_x - I_t^{\alpha}\left[R_{21}(t - \tau_{rel})\varepsilon_x\right] + \varepsilon_y - I_t^{\alpha}\left[R_{22}(t - \tau_{rel})\varepsilon_y\right] + \varepsilon_z - I_t^{\alpha}\left[R_{23}(t - \tau_{rel})\varepsilon_z\right], \tag{5}$$

$$\sigma_z = \varepsilon_x - I_t^{\alpha}\left[R_{31}(t - \tau_{rel})\varepsilon_x\right] + \varepsilon_y - I_t^{\alpha}\left[R_{32}(t - \tau_{rel})\varepsilon_y\right] + \varepsilon_z - I_t^{\alpha}\left[R_{33}(t - \tau_{rel})\varepsilon_z\right], \tag{6}$$

$$\tau_{xy} = \gamma_{xy} - I_t^{\alpha}\left[R_{44}(t - \tau_{rel})\gamma_{xy}\right], \tag{7}$$

$$\tau_{xz} = \gamma_{xz} - I_t^{\alpha}\left[R_{55}(t - \tau_{rel})\gamma_{xz}\right], \tag{8}$$

$$\tau_{yz} = \gamma_{yz} - I_t^{\alpha}\left[R_{66}(t - \tau_{rel})\gamma_{yz}\right] \tag{9}$$

where $R_{ij}(t - \tau_{rel})$ - relaxation kernels tensor.

We introduce a notation to simplify further description of the material

$$D_{xy}^{2\alpha} f(x, y) = D_x^{\alpha}\left(D_y^{\alpha} f(x, y)\right). \tag{10}$$

Considering (3), the ratio of the deformation community in biomaterials with a fractal structure were follows

$$D_{yy}^{2\alpha} \varepsilon_x + D_{xx}^{2\alpha} \varepsilon_y = D_{xy}^{2\alpha} \gamma_{xy}, \tag{11}$$

$$D_{zz}^{2\alpha} \varepsilon_x + D_{xx}^{2\alpha} \varepsilon_z = D_{xz}^{2\alpha} \gamma_{xz}, \tag{12}$$

$$D_{zz}^{2\alpha} \varepsilon_y + D_{yy}^{2\alpha} \varepsilon_z = D_{yz}^{2\alpha} \gamma_{yz}, \tag{13}$$

$$\frac{1}{2} D_x^{\alpha}\left(D_y^{\alpha} \gamma_{xz} + D_z^{\alpha} \gamma_{xy} - D_x^{\alpha} \gamma_{yz}\right) = D_{yz}^{2\alpha} \varepsilon_x, \tag{14}$$

$$\frac{1}{2} D_y^{\alpha}\left(D_z^{\alpha} \gamma_{xy} + D_x^{\alpha} \gamma_{yz} - D_y^{\alpha} \gamma_{xz}\right) = D_{xz}^{2\alpha} \varepsilon_y, \tag{15}$$

$$\frac{1}{2} D_z^{\alpha}\left(D_x^{\alpha} \gamma_{yz} + D_y^{\alpha} \gamma_{xz} - D_z^{\alpha} \gamma_{xy}\right) = D_{xy}^{2\alpha} \varepsilon_z. \tag{16}$$

So, using this approach we can obtain the viscoelastic deformation problem with taking into account the fractal structure of the biomaterial.

2.2. Variational formulation of the viscoelastic deformation problem

Particular interest has direction of obtaining continuous solutions of stress-strain state problem in biomaterials with a fractal structure. This becomes possible with using variational formulations of such problems. The principle of virtual works is widely used for this purpose.

All general theorems for small deformations is based on the equation of virtual works [1, 35]

$$\iiint_V \boldsymbol{\sigma}_{ij}\boldsymbol{\varepsilon}_{ij}dV = \iiint_V \rho\overline{\mathbf{F}}_i\mathbf{u}_i dV + \iint_S \overline{\mathbf{F}}_{V\,i}\mathbf{u}_i dS. \tag{17}$$

where V - body volume, S - body surface.

Thus, among all permissible displacements u,υ,ω that satisfy the boundary conditions, the active displacements result in a stationary of full potential energy and provide a minimum of functional Π

$$\Pi = \iiint_V [A(u,\upsilon,\omega)+\Phi(u,\upsilon,\omega)]dV + \iint_S \Psi(u,\upsilon,\omega)dS, \tag{18}$$

$$-\Phi(u,\upsilon,\omega) = \rho\overline{X}u + \rho\overline{Y}\upsilon + \rho\overline{Z}\omega, \tag{19}$$

$$-\Psi(u,\upsilon,\omega) = \overline{X}_V u + \overline{Y}_V\upsilon + \overline{Z}_V\omega, \tag{20}$$

where $A(u,\upsilon,\omega)$ - the strain energy function can be written in the form

$$\begin{aligned} A(u,\upsilon,\omega) = {} & \left(div^\alpha\mathbf{u}\right)^2 - \Big(D_x^\alpha u * I_t^\alpha\left[R_{11}(t-\tau_{rel})D_x^\alpha u + R_{12}(t-\tau_{rel})D_y^\alpha\upsilon + R_{13}(t-\tau_{rel})D_z^\alpha\omega\right] + \\ & D_y^\alpha\upsilon * I_t^\alpha\left[R_{21}(t-\tau_{rel})D_x^\alpha u + R_{22}(t-\tau_{rel})D_y^\alpha\upsilon + R_{23}(t-\tau_{rel})D_z^\alpha\omega\right] + \\ & D_z^\alpha\omega * I_t^\alpha\left[R_{31}(t-\tau_{rel})D_x^\alpha u + R_{32}(t-\tau_{rel})D_y^\alpha\upsilon + R_{33}(t-\tau_{rel})D_z^\alpha\omega\right]\Big) + \\ & \left(\left(D_y^\alpha u + D_x^\alpha\upsilon\right)^2 + \left(D_y^\alpha u + D_x^\alpha\upsilon\right)^2 + \left(D_z^\alpha\upsilon + D_y^\alpha\omega\right)^2\right) - \\ & \Big(\left(D_y^\alpha u + D_x^\alpha\upsilon\right) * I_t^\alpha\left[R_{44}(t-\tau_{rel})\left(D_y^\alpha u + D_x^\alpha\upsilon\right)\right] + \\ & \left(D_z^\alpha u + D_x^\alpha\omega\right) * I_t^\alpha\left[R_{55}(t-\tau_{rel})\left(D_z^\alpha u + D_x^\alpha\omega\right)\right] + \\ & \left(D_z^\alpha\upsilon + D_y^\alpha\omega\right) * I_t^\alpha\left[R_{66}(t-\tau_{rel})\left(D_z^\alpha\upsilon + D_y^\alpha\omega\right)\right]\Big) \end{aligned} \tag{21}$$

$$div^\alpha\mathbf{u} = D_x^\alpha u + D_y^\alpha\upsilon + D_z^\alpha\omega. \tag{22}$$

Substitute the expression of stresses due to deformations from the relations (4)-(9). Then, taking into account relation (3), the equilibrium conditions on the surface due to displacement was obtained

$$\begin{aligned} \overline{X}_V = {} & \left(div^\alpha\mathbf{u} - I_t^\alpha\left[R_{11}(t-\tau_{rel})D_x^\alpha u\right] - I_t^\alpha\left[R_{12}(t-\tau_{rel})D_y^\alpha\upsilon\right] - I_t^\alpha\left[R_{13}(t-\tau_{rel})D_z^\alpha\omega\right]\right)\cos(n,x) + \\ & \left(\left(D_y^\alpha u + D_x^\alpha\upsilon\right) - I_t^\alpha\left[R_{44}(t-\tau_{rel})\left(D_y^\alpha u + D_x^\alpha\upsilon\right)\right]\right)\cos(n,y) + \\ & \left(\left(D_z^\alpha u + D_x^\alpha\omega\right) - I_t^\alpha\left[R_{55}(t-\tau_{rel})\left(D_z^\alpha u + D_x^\alpha\omega\right)\right]\right)\cos(n,z) \end{aligned} \tag{23}$$

$$\begin{aligned} \overline{Y}_V = {} & \left(div^\alpha\mathbf{u} - I_t^\alpha\left[R_{21}(t-\tau_{rel})D_x^\alpha u\right] - I_t^\alpha\left[R_{22}(t-\tau_{rel})D_y^\alpha\upsilon\right] - I_t^\alpha\left[R_{23}(t-\tau_{rel})D_z^\alpha\omega\right]\right)\cos(n,y) + \\ & \left(\left(D_y^\alpha u + D_x^\alpha\upsilon\right) - I_t^\alpha\left[R_{44}(t-\tau_{rel})\left(D_y^\alpha u + D_x^\alpha\upsilon\right)\right]\right)\cos(n,x) + \\ & \left(\left(D_z^\alpha\upsilon + D_y^\alpha\omega\right) - I_t^\alpha\left[R_{55}(t-\tau_{rel})\left(D_z^\alpha\upsilon + D_y^\alpha\omega\right)\right]\right)\cos(n,z) \end{aligned} \tag{24}$$

$$\begin{aligned} \overline{Z}_V = {} & \left(div^\alpha\mathbf{u} - I_t^\alpha\left[R_{31}(t-\tau_{rel})D_x^\alpha u\right] - I_t^\alpha\left[R_{32}(t-\tau_{rel})D_y^\alpha\upsilon\right] - I_t^\alpha\left[R_{33}(t-\tau_{rel})D_z^\alpha\omega\right]\right)\cos(n,z) + \\ & \left(\left(D_z^\alpha u + D_x^\alpha\omega\right) - I_t^\alpha\left[R_{44}(t-\tau_{rel})\left(D_z^\alpha u + D_x^\alpha\omega\right)\right]\right)\cos(n,x) + \\ & \left(\left(D_z^\alpha\upsilon + D_y^\alpha\omega\right) - I_t^\alpha\left[R_{55}(t-\tau_{rel})\left(D_z^\alpha\upsilon + D_y^\alpha\omega\right)\right]\right)\cos(n,y) \end{aligned} \tag{25}$$

Thus, a variational formulation of the viscoelastic deformation problem of biomaterials with a fractal structure was obtained.

3. Software for calculating the dynamics of the stress-strain state components of biomaterials with a fractal structure

For finding a numerical solution to the problem of viscoelastic deformation of biomaterials with a fractal structure in the process of heat treatment application software was developed in the programming language GNU Octave 5.2.0.

When finding a numerical solution of the problem, the main advantages of the Octave environment were as follows:

- a large number of built-in functions for finding solutions of interpolation and approximation problems;
- a wide range of statistical functions of statistical regression and other functions of mathematical statistics and analysis of experimental data;
- a specially designed class that allows you to work with sparse matrices.

A usecase diagram was constructed of developed software for finding the numerical solution of viscoelastic deformation problem of biomaterials with a fractal structure in the process of heat treatment, which is shown in Fig. 1.

As you can see, the user has the following options when finding a solution to the problem of viscoelastic deformation: "Set the rheological parameters of the biomaterial", "Choose the sample type", "Set modeling time", "Set the geometric sizes of the sample", "Set the initial value", "Set the boundary conditions", "Compute the stress-strain problem","Set the parameters of numerical method". Option of usecase "Compute the stress-strain problem" - implements the algorithm for finding the numerical solution of the problem (18)-(25). Execution of this usecase variant leads to automatic execution of the following: "Determine the strain modulus", "Calculate the relaxation function".

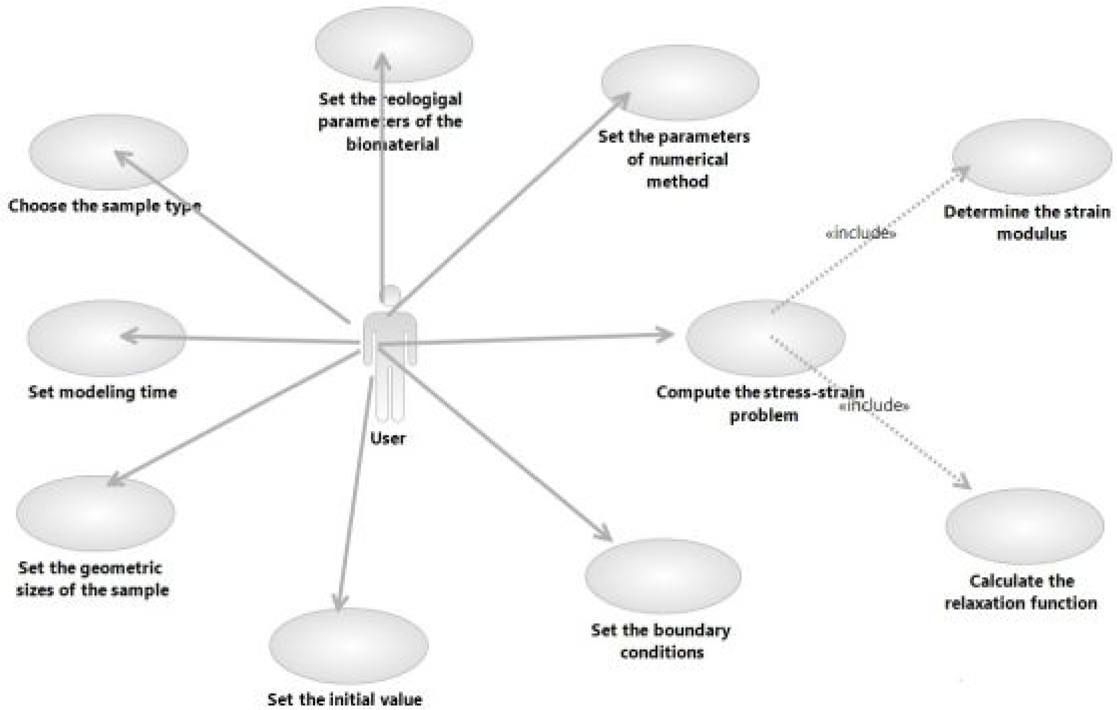

Figure 1: Usecase diagram of developed software for finding the numerical solution of viscoelastic deformation problem of biomaterials with fractal structure

In Fig. 2 shows a sequence diagram constructed for the "Compute the stress-strain problem" usecase. It reflects the sequence of actions performed to find a numerical solution to the problem of viscoelastic deformation of biomaterials with a fractal structure in the process of heat treatment.

This usecase uses the functionality of the UserForm and Solver objects. The UserForm object is designed to specify the user: modeling time, type of biomaterials, geometric dimensions, initial values of stresses and strains, parameters of the numerical method and setting the rheological parameters of the mathematical model of viscoelastic deformation of biomaterials in heat treatment.

The Solver object is designed to implement an algorithm for finding a numerical solution to the problem of viscoelastic deformation of biomaterials with a fractal structure in the heat treatment process. It contains methods that allow to determine the values of instantaneous module of elasticity, calculate the relaxation function, implement a numerical method, build graphical dependences of the dynamics of stress and strain components on the sample depending on time and spatial coordinates.

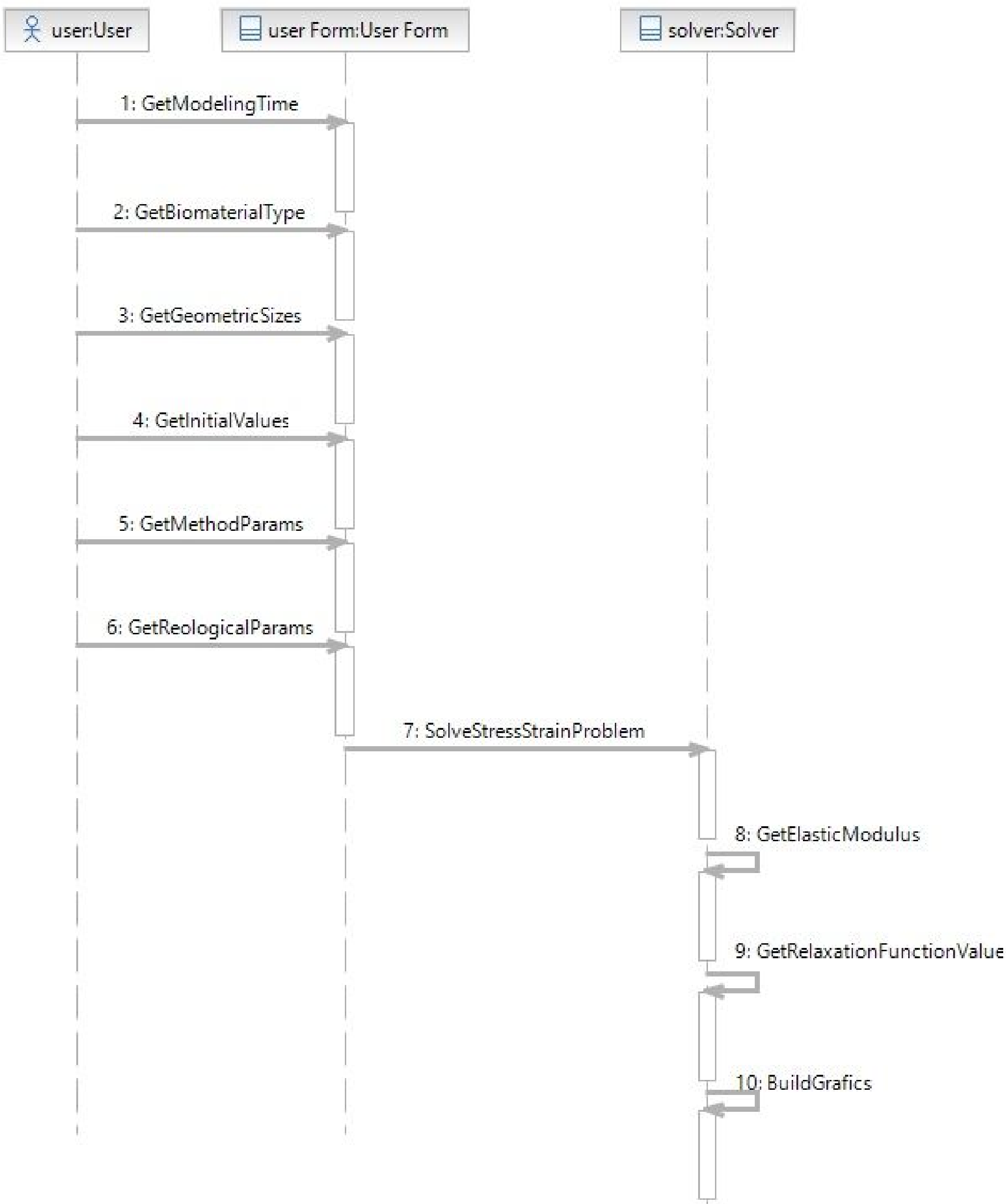

Figure 2: Sequence diagram for the use of "Compute the stress-strain problem" usecase

The Solver object also contains methods that allow you to control the process of finding the numerical solution of the viscoelastic deformation problem:

- SolveStressStrainStateProblem - implementation of the algorithm for finding the numerical solution of the model;
- GetElasticModulusValues - calculation of values of instantaneous modulus of elasticity;
- GetRelaxationFunctionValue - calculation of the value of the relaxation function;
- BuildGrafics - construction of graphical dependences of dynamics of components of stresses and strains.

4. Obtained results

During the process of heat treatment of biomaterials the moisture content in the central layers increases and in the surface - decreases. This leads to the appearance of stresses of different signs: in the surface layers - positive; in the central - negative. Let us investigate the dependences of the stress components σ_x and σ_y dynamics within 48 hours. We show the difference between the values of the stress components obtained by implementing a mathematical model of viscoelastic deformation of biomaterials with taking into account the fractal structure during heat treatment and without. To take into account the fractal structure of the material the fractional derivative index α is set equal to the value determined by approximating the experimental data. Values $\alpha = 1$ are set to neglect the fractal structure of the material.

The results of realization of the mathematical model of viscoelastic deformation of biomaterials with fractal structure depending on the geometric dimensions of the sample are considered. A biomaterial with the following values of physical parameters of the material was selected for the numerical experiment: base density - $\rho = 560$ kg/m^3, ambient temperature - $t_c = 70\ {}^0C$. Cross-section points of the biomaterial will be used to compare the numerical values of the simulated processes. l_1 and l_2 is half of the sample size. The point $A(0;0)$ is in the center of the pattern, the point $B(l_1/2; l_2/2)$ is in the middle, $C(l_1; l_2)$ is in the corner of the rectangular pattern.

In Fig. 3 and Fig. 4 shows the dynamics of the stress components at the point $C(l_1; l_2)$ of the sample during 48 hours of heat treatment. It can be seen that by changing the proportional relationships between the lengths of the surface of the sample the nature of the stress curves changes significantly. In particular, this is observed with a change in the proportions from $l_2/l_1 = 3$ to $l_2/l_1 = 2$.

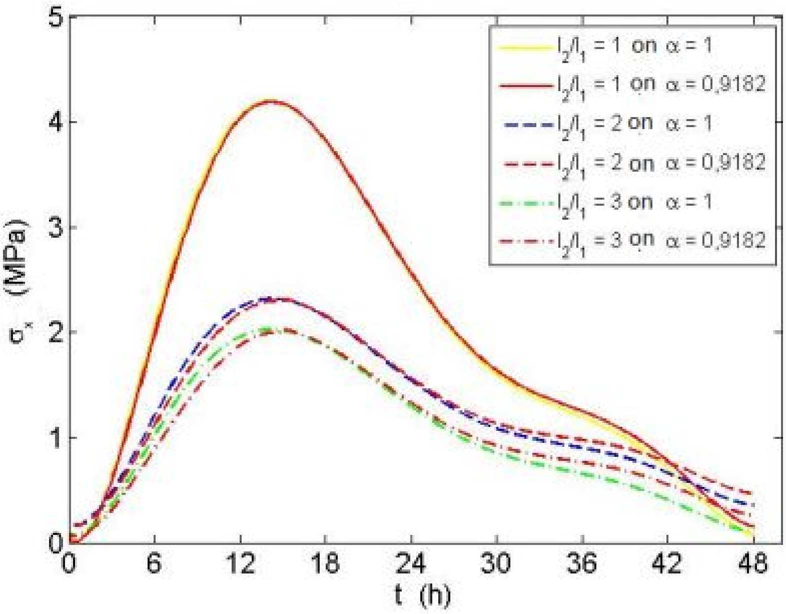

Figure 3: Changing of the stress component σ_x at a point $C(l_1; l_2)$ on the sample depending on its geometric dimensions

Analyzing the behavior of the curves in Fig. 3 and Fig. 4 can be concluded that with increasing the ratio between the sides of the sample, the fractal structure of the material has a more significant effect on the dynamics of stress components and residual stresses. In particular, we can see that the difference between the stresses with taking into account the fractal structure and without at $l_2/l_1 = 1$ does not exceed 4.1%, at $l_2/l_1 = 2 - 8.4\%$, at $l_2/l_1 = 3$ $- 15.7\%$.

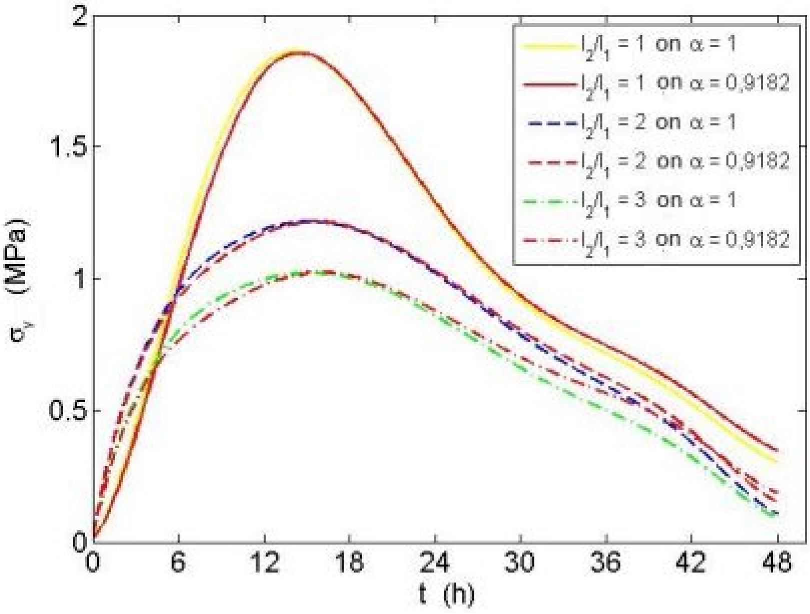

Figure 4: Changing of the stress component σ_y at a point $C(l_1;l_2)$ on the sample depending on its geometric dimensions

Graphic dependence in Fig. 5 shows the dynamics of stress components in biomaterials depending on its type. In particular, we consider a biomaterial of type №1, denote its biomat1, with a base density equal to $\rho = 680$ kg/m^3, biomat2 - with a density of $\rho = 625$ kg/m^3, biomat3 - with a density of $\rho = 480$ kg/m^3.

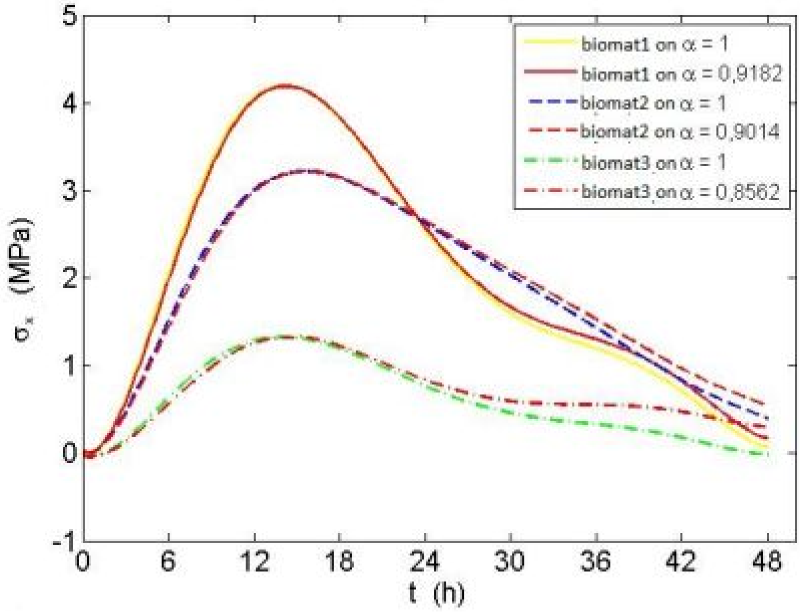

Figure 5: Changing of the stress component σ_x at a point $C(l_1;l_2)$ on the sample depending on biomaterial type

We can conclude that for biomaterials with approximately the same density, the stresses differ by no more than 12.5%. Instead, for materials with lower density the stress dynamics is different. The numerical values of the stress components in such materials are several times smaller. However, the type of stresses dymanics in all samples remains the same.

5. Conclusions

Using the basic laws of mechanics of hereditary environments and the mathematical apparatus of integro-differentiation of fractional order, new mathematical models of viscoelastic deformation of biomaterials with fractal structure in the process of heat treatment were obtained, which allows to take into account the complex nature of spatial correlations and deterministic chaos.

The basic equations of viscoelastic deformation of biomaterials taking into account their fractal structure are obtained. A variational formulation of the viscoelastic deformation problem of biomaterials with taking into account their fractal structure is obtained. Which allows to obtain an approximate continuous solution of the problem.

Application software for finding an approximate solution of the viscoelastic deformation problem of biomaterials with taking into account their fractal structure was developed. The usecase diagram of the developed software and the sequence diagram for usecase which provides reception of a numerical decision were constructed.

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