Modeling of Heat Transfer and Deformation Processes in Biomaterials with Fractal Structure

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Abstract

The theoretical foundations of the study of deformation-relaxation and heat exchange processes in biomaterials with a fractal structure based on the synthesis of the basic laws of thermodynamics of nonequilibrium processes and mechanics of a continuous medium were further developed. A new physical and mathematical model of interconnected deformable and heat exchange processes in biomaterial with taking into account its fractal structure depending on viscoelastic characteristics was synthesized. To take into account the fractal structure of the material the mathematical apparatus of integro-differentiation of fractional order was used. For the partial case, the numerical values of the simulated physical characteristics were obtained. The obtained results were analysed and conclusions were made about the distribution and influence of interconnected heat exchange and deformation relaxation processes in biomaterials with taking into account their fractal structure.

Keywords 1

Fractal structure, biomaterial, deformation-relaxation processes, heat transfer, total energy

1. Introduction

In general uneven fuel expansion cannot occur freely in a solid body and causes thermal (thermal, temperature) stresses. Knowledge of the magnitude and nature of the thermal stresses effect is necessary for a comprehensive analysis of the structural strength. The action of mechanical stresses from external forces and in combination with thermal loads can cause cracks and destruction of structures that have been made of materials with a complex structure [1-5].

With the rapid appearance of stresses due to the action of a sharp gradient of an unsteady temperature field some materials become brittle and cannot withstand thermal shock. Repeated application of thermal loads leads to an overload of structural elements [6].

In the general case, a change in body temperature occurs not only due to the supply of heat from external sources but also due to the deformation process itself. Thermomechanical effects of a different kind are important in deformations of a body that are flowing at a finite speed: the formation and movement of heat flow inside the body, the appearance of bound elastic and heatwaves in it, and thermoelastic energy dissipation [7, 8].

Most real physical processes cannot be described using the basic principles and concepts of the mechanics of a continuous medium. This requires the involvement of non-traditional approaches, in

IDDM'2021: 4rd International Conference on Informatics & Data-Driven Medicine, November 19–21, 2021, Valencia, Spain
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particular, the fractality of the environment in which these processes take place. Superslow diffusion-type processes, deformation-relaxation processes in the middle with obvious memory effects can be brought to such processes. To describe them in the proper way the accordingly modified laws are used, which require the implementation of the fractional integro-differential mathematical apparatus [9-11].

Fractional mathematical analysis has a long history, but despite this, it is a rapidly developing area of modern analysis and has extremely rich content. At present, there is not a single area of classical analysis that has not been touched by fractional analysis, which is closely related to various issues of the theory of functions, integral and differential equations, mechanics, equations of mathematical physics, etc. The mathematical language of operators of fractional integro-differentiation is indispensable for describing and researching physical fractal systems, stochastic transfer processes, the study of mechanics, biology, probability theory and other applied sciences [12-15].

It is necessary to take into account the internal structure and properties of materials during constructing mechanical and mathematical models. It is very important to build mathematical models that describe the stress-strain state and thermoelasticity in media that “do not fit into the traditional approach” of known and developed standard mathematical models of specific branches of mechanics of continuous media. So, for example, the use of classical models of elastic bodies deformation in bio/nanomechanics without taking into account the complicated structure of biomaterials does not allow to obtain reliable results and sharply narrows the scope of the problems being solved [16-21].

At the same time to obtain the results of higher accuracy by improving and complicating the algorithms for the numerical implementation of the tasks is almost impossible.

Thus, to obtain adequate results for modeling the behavior of real physical objects, it is necessary to change the approach when building a mathematical model. Construction of basic equations of mechanics using the apparatus of fractional calculus to describe the behaviour of real heterogeneous materials is one of the promising areas for further improvement and development of mechanical and mathematical models [22-24, 9, 12].

Thus, the study of the thermomechanical characteristics of porous biomaterials, which are characterized by the complex nature of the spatial structure, existing memory effect, self-organization and deterministic chaos properties, is an urgent scientific task.

2. Production of a problem

Many definitions of derivatives and fractional integrals are known today, in particular: Caputo, Marshaud, Weil and others. All these operators of fractional integro-differentiation have a rather cumbersome construction and can take various forms is the actions on which do not always coincide. On the other side, it is impossible to firmly assert which of the approaches is advisable to study and which is not since there is no unambiguous definition of derivatives of non-integer order. The mathematical apparatus of integro-differentiation of fractional order was used in the construction of mathematical models of the studied physical processes occurring in biomaterials with a fractal structure. In particular, the integral and the derivative of the function $f(x,y,z)$ by the variable x in the Caputo’s sense can be written as follows [10, 12-15, 22]:

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

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

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. Determination of internal and free energy of deformation and heat exchange processes

The purpose of this section was to build theoretical foundations and develop methods for the synthesis of deformation-relaxation processes in biomaterials with a fractal structure during their heat treatment. Biomaterial, in particular bone, is considered to be an open thermodynamic system with a variable volume [1, 2, 6].

Let's select an infinitesimal element of material in the Cartesian coordinate system. Its state is characterized by a system of independent variables $S, \varepsilon_{ij}, U_{ij}$, or equivalent system $T, \varepsilon_{ij}, U_{ij}$, where S is the entropy of a unit of mass; T - absolute temperature; ε_{ij} - components of the strain tensor; ρ - density of the material; τ - time; $J = \{J_{ijk}\}$ - tensor of the third rank which characterizes the corresponding thermodynamic flow and satisfies the balance equation:

$$divJ = 0 \tag{3}$$

The relationship between deformations and displacements that take into account the fractal structure of the biomaterial is recorded using modified Cauchy relations:

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \tag{4}$$

$$u_{i,j} = D_{x_j}^{\alpha} u_i \tag{5}$$

The thermodynamic potential of the described system in case of temperature change is free energy. The full differential of free energy can be written in the form [25]:

$$dF = dF_0 + dF_1, \tag{6}$$

$$dF_0 = -SdT, \tag{7}$$

$$dF_1 = \rho\sigma_{ij} d\varepsilon_{ij} + \chi_{ij} d\omega_{ij}, \tag{8}$$

where, σ_{ij} - components of the stress tensor; ω_{ij} - components of the damage tensor; χ_{ij} - corresponding potential. Thus, the full differential of free energy can be written as [25]:

$$dU = -TdS + \rho\sigma_{ij} d\varepsilon_{ij} + \chi_{lm} d\omega_{lm} \tag{9}$$

For small deviations of the system from the equilibrium state, the free energy, expressed in terms of temperature, stress tensors, deformations and damages, is a complete differential and can be represented as:

$$F\left(T, \varepsilon_{ij}, \omega_{lm}\right) = F_0 + \frac{\partial F_0}{\partial \varepsilon_{ij}} \varepsilon_{ij} + \frac{1}{2} \frac{\partial^2 F_0}{\partial \varepsilon_{ij} \varepsilon_{lm}} \varepsilon_{ij} \varepsilon_{lm} \tag{10}$$

At the initial moment, the equilibrium state is characterized by the initial conditions:

$$S = S_0,\ T = T_0,\ \sigma_{ij} = 0,\ \varepsilon_{ij} = 0. \tag{11}$$

For the free energy function, the Taylor series expansion according to the degrees of deformation invariants is valid. Restricted to members not higher than the second order, we obtain:

$$F = F_0\left(T, r_0\right) + \frac{\partial F_0}{\partial I_1} I_1 + \frac{\partial F_0}{\partial I_2} I_2 + \frac{1}{2} \frac{\partial^2 F_0}{\partial I_1^2} I_1^2 \tag{12}$$

$$I_1 = \varepsilon_{ii};\ I_2 = \varepsilon_{ij}\varepsilon_{ij} \tag{13}$$

Given the generalization of Hooke's law for materials with a fractal structure in the presence of viscoelastic deformations:

$$F = c_v \frac{dT}{dT_0} + \varepsilon_{ij}\varepsilon_{ij}\left(1 - \omega\right) + \varepsilon_{ij}^2\left(\frac{\lambda}{2} + \frac{\mu\omega}{3}\right) - \varepsilon_{ij} \frac{dV}{V_0}\left(2\mu + 3\lambda\right) \tag{14}$$

$$\sigma_{ij} = 2\mu\left(1 - \omega\right)\varepsilon_{ij} + \left[\varepsilon_{ij}\left(\lambda + \frac{2}{3}\mu\omega\right) - \frac{dV}{V_0}\left(3\lambda + 2\mu + \zeta P\right)\right]\delta_{ij} \tag{15}$$

$$S = c_v \frac{dT}{dT_0} + \varepsilon_{ij} \frac{\partial}{\partial T}\left[\frac{dV}{V_0}(2\mu + 3\lambda) + \zeta P\right] + \varepsilon_{ij}\varepsilon_{ij} \frac{\partial}{\partial T}[\mu(1-\omega)] + \varepsilon_{ij}^2 \frac{\partial}{\partial T}\left(\frac{\lambda}{2} + \frac{\mu\omega}{3}\right) \quad (16)$$

where ζ - is determined based on measuring the pressure and the correspondence of the change in specific volume in the region of elastic deformations at a constant temperature.

2.2. Synthesis of a model of deformation and heat exchange processes in a biomaterial with a fractal structure

To obtain a system of equations that describe the interrelated deformation-relaxation and heat exchange processes in biomaterials with a fractal structure it is necessary to obtain the equation of energy and motion balance. According to the first law of thermodynamics the total energy U^* of a volume V limited by a surface Ω is determined by the ratio [4, 5]:

$$U^* = \int_V \rho U dV + \frac{1}{2}\int_V \rho \overline{V}^2 dV \quad (17)$$

where $\overline{V}$ - velocity, U - the density of internal energy per unit volume of deformed biomaterial.

The work of external forces over some time with taking into account the available memory effect can be described [25]:

$$\delta A = I_\tau^\alpha\left[\int_V \rho(FV)dV\right] + \int_\Omega \left(\overline{\sigma_n}\overline{V_n}\right)d\Omega \quad (18)$$

$$\overline{\sigma_n} = \sigma_i \cos(nx_i) \quad (19)$$

where $\overline{\sigma_n}$ is the vector of normal stresses to the surface; n - normal to the surface Ω.

The total flow of thermal energy over some time due to the action of an internal source q and heat input is determined by the ratio [25]:

$$\delta Q^* = I_\tau^\alpha\left[\int_V q dV\right] - \int_\Omega \overline{S_n} d\Omega \quad (20)$$

$$\overline{S_n} = S_i \cos(nx_i) \quad (21)$$

In the case of internal heat sources, we obtain:

$$\Delta U^* = I_\tau^\alpha\left[\int_V \rho(FV)dV\right] + \int_\Omega \left(\overline{S_n} - \overline{\sigma_n}\overline{V_n}\right)d\Omega \quad (22)$$

When considering an infinitesimal period, ie $\Delta\tau \to 0$, we can write the following relationship:

$$D_\tau^\alpha\left[\int_V \rho\left(U + \frac{\overline{V}^2}{2}\right) - \rho(FV)dV\right] + \int_\Omega \rho\left(\overline{S_n} - \overline{\sigma_n}\overline{V_n}\right)d\Omega = 0 \quad (23)$$

Applying Green's formula and taking into account the arbitrariness of the volume we get:

$$\rho D_\tau^\alpha U = -J_{i,i} + \overline{\sigma_i}\overline{V_i} - \rho\left(\overline{F^i}\,\overline{V}\right) \quad (24)$$

Given that the components of the strain tensor and strain rates are interrelated, the expression for the increase in internal energy per unit mass and unit time depending on the temperature and strain fields can be written:

$$\rho D_\tau^\alpha U = -J_{i,i} + \sigma_{ij} D_\tau^\alpha e_{ij} \quad (25)$$

Using (9) the equation of entropy balance will be written in the form

$$\rho T D_\tau^\alpha S = \rho D_\tau^\alpha U - \sigma_{ij} D_\tau^\alpha e_{ij} - \rho\mu_{ij} D_\tau^\alpha e_{ij} \quad (26)$$

Given (25) the equation of state will be written:

$$\rho T D_\tau^\alpha S = -J_{i,i} + \mu_{ij} J_{kij,k} \quad (27)$$

Using the specific heat of the material of the relationship (26) can be written as:

$$\rho c_v D_\tau^\alpha T + TD_\tau^\alpha \left[\varepsilon_{ii} \frac{\partial}{\partial T} \left(\frac{dV}{V_0} (2\mu + 3\lambda) + \zeta P \right) \right] = -J_{i,i} + \mu_{ij} J_{kij,k} \tag{28}$$

From relation (27) we obtain the definition of thermodynamic forces of energy transfer:

$$\rho TD_\tau^\alpha S = J_i + J_i X_i + J_{ijk} X_{jki} \tag{29}$$

$$X_i = -\frac{T_{i,i}}{T} \tag{30}$$

Thus, the equations combining thermodynamic flows will look like this:

$$J_{ij} = \lambda T_{ij,ji} \tag{31}$$

$$J_i = -L_{TT} \frac{T_{i,i}}{T} \tag{32}$$

Taking into account the above relations, the physical-mathematical model of interconnected heat exchange and deformation processes in biomaterials with a fractal structure during their heat treatment is synthesized.

$$\sigma_{ij,i} = \rho D_\tau^{2\alpha} u_i - \rho F \tag{33}$$

$$\frac{\lambda}{\rho c_v} T_{ij,ji} = D_\tau^\alpha T + TD_\tau^\alpha \left[\varepsilon_{kk} \frac{\partial}{\partial T} G(T,P) \right] \tag{34}$$

$$D_\tau^\alpha P = a_P \Delta^2 P + \frac{1}{\rho C} T_{ij,ji} - PD_\tau^\alpha \left[\varepsilon_{kk} \frac{\partial}{\partial P} G(T,P) \right] \tag{35}$$

$$G(T,P) = \frac{dV}{V_0} (3\lambda + 2\mu) - 3P \tag{36}$$

To relations (33) - (36) are also added (15), (16), kinematic equations (31) - (32) and geometric (4). Thus, these equations form a physic-mathematical model for calculating the interconnected heat transfer and deformation processes in biomaterials with a fractal structure from the time of their heat treatment.

3. Obtained results

The biomaterials tend to expand during the heat treatment process. This fact encourages the appearance of stresses in the material. Let us consider a numerical experiment for the obtained model, which is designed to investigate the effect of heat load and the degree of fractality of the material on the maximum modulus of stress values in it [26, 27].

A numerical experiment [28] is given for bone material with the initial value of temperature $T_0 = 36.6\ ^0C$. The bone material was taken as a sample with the following geometric dimensions $x \in [0; l]$, where $l = 0.15$ - the length of the sample. The interaction of the studied biomaterial with external thermal loads is given by the boundary conditions, in particular, the impermeability condition is set at the left boundary $x = 0$, and the interaction with the medium that has a temperature $t_c = 60\ ^0C$ is set at the right boundary $x = l$ [29, 30, 11]. The hypothesis of a natural stress state, the absence of stresses, deformations and displacements in the material at the initial time is accepted ($\sigma_{11}|_{\tau=0} = 0;\ \varepsilon_{11}|_{\tau=0} = 0;\ u|_{\tau=0} = 0$). Also, the material is not subject to any mechanical stress [31, 32].

Fig. 1 shows the dynamics of temperature change in bone material during 2 hours exposed to heat flux, the nature of which is described above. The curve corresponding to the parameter $\alpha = 1$ shows the dynamics of temperature change calculated using the traditional approach. The curves corresponding to the parameters $\alpha = 0.95$ and $\alpha = 0.9$ represent the dynamics of temperature change, calculated using the apparatus of integro-differentiation of fractional order, i.e. take into account the fractal structure of the medium. Fig. 2 shows the dynamics of normal stress σ_{11} over 2 hours, which occurs in the material due to the action of heat fluxes.

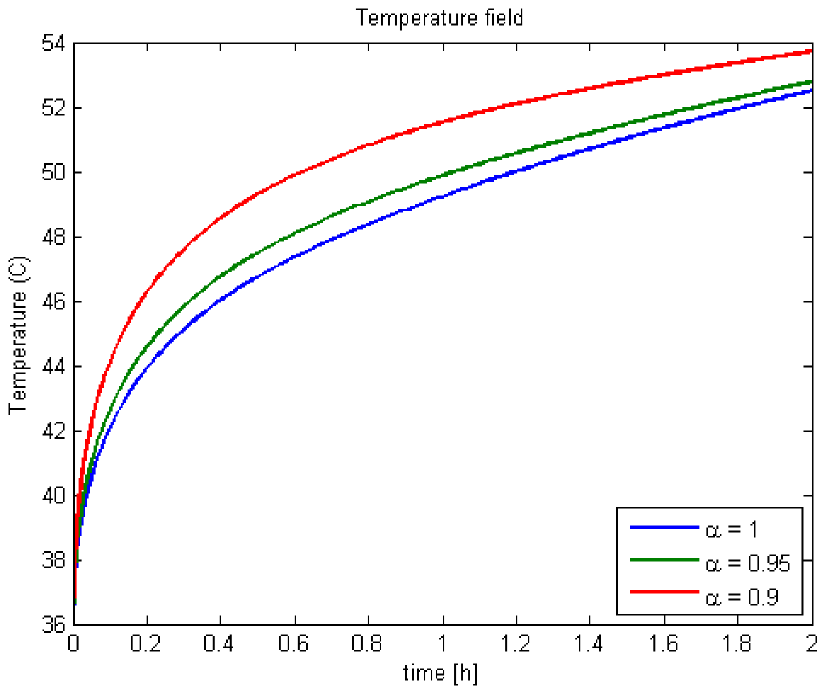

Figure 1: Changing of the temperature at the right boundary $x = l$ on the sample depending on time and fractional degree of material

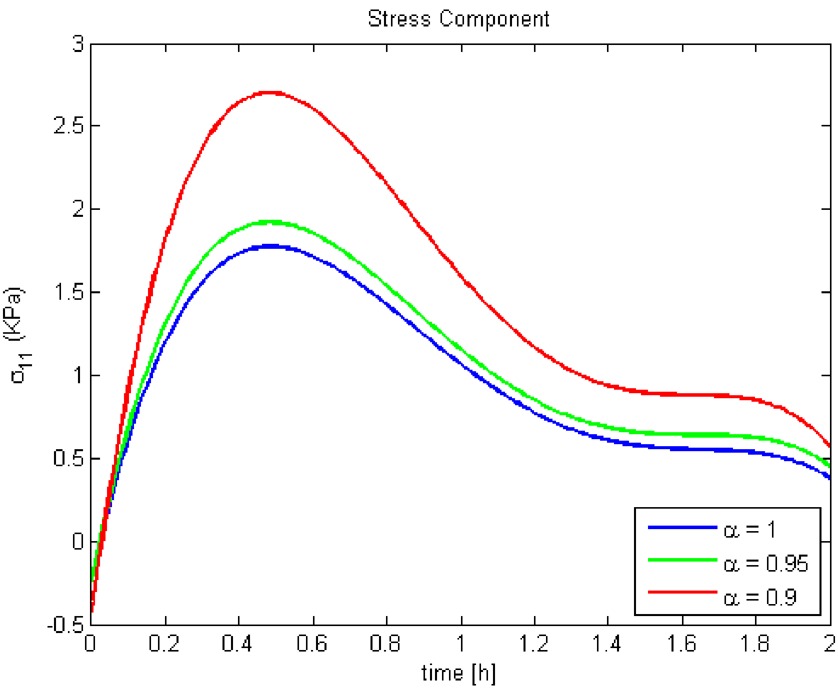

Figure 2: Changing of the stress component σ_{11} at the right boundary $x = l$ on the sample depending on time and fractional degree of material

Analysing the behaviour of the curves in Fig. 1 and Fig. 2 can be concluded that the rate of its heating increases with the increasing degree of fractality of the material. In particular, the maximum difference between the temperatures of the material with taking into account the fractal structure $\alpha = 0.95$ and without $\alpha = 1$ is equal $0.78\ ^{o}C$, and for the material with the degree of fractality $\alpha = 0.9$ - is $2.27\ ^{o}C$.

The temperature changing in the material leads to stresses in it. The higher in the absolute value stresses appear when the faster temperature changes. In particular, the maximum difference between the components of the normal stress σ_{11} of the material with taking into account the fractal structure $\alpha = 0.95$ and without $\alpha = 1$ is equal $0.21 KPa$, and for a material with a degree of fractality $\alpha = 0.9$ - is $1.07 KPa$. It can also be noted that with increasing degree of fractality of the material increases the value of residual stresses that have a significant impact on the development of stresses in the material when applying to it repeated thermal or mechanical loads.

4. Conclusions

The use of the mathematical apparatus of integro-differentiation of fractional order allows creating a new basis for the further development of the theoretical foundations of the study of deformation-relaxation and heat exchange processes in biomaterials with a fractal structure. The synthesized physical-mathematical model of interconnected deformable and heat-exchange processes allows to describe the rheological behaviour of biomaterial in the process during its heat treatment with taking into account available memory effects, self-organization and deterministic chaos depending on viscoelastic characteristics.

After analysing the obtained numerical results for partial cases, we can conclude that in heat treatment processes biomaterials with a higher degree of fractality heat up faster, which leads to the presence of higher absolute values of stresses. This fact leads to the accumulation of residual stresses, which significantly affect the development of stresses in the material when applying to it repeated thermal or mechanical loads.

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