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10. PARAMETRIC IDENTIFICATION AND MODELING OF RHEOLOGICAL BEHAVIOR OF MATERIALS WITH FRACTAL STRUCTURE DURING HEAT TREATMENT

The technological process of thermal treatment of capillary-porous materials, characterized by the influence of several factors on the material as load, humidity and temperature was considered. Mathematical models of non-isothermal moisture transfer and viscoelastic deformation, taking into account the fractal structure of the environment were constructed. One-dimensional mathematical models of deformation-relaxation processes in environments with fractal structure characterized by the effects of memory, spatial nonlocality and self-organization were considered. Taking into account that the fractional parameters of fractal models allow us to describe the deformation-relaxation processes in comparison with traditional methods more fully, the optimal approximation method, the Proni's method was proposed. This method allows us to reduce the problem of identification of the fractional parameters which are 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.

10.1. INTRODUCTION

Investigation of deformation-relaxation processes have shown that using fractional integrate-differential apparatus for modeling those processes allows the implementation of experimental data to identify model parameters [3, 5, 7] more appropriately on the basis of physical considerations. Particularly important are the works devoted to research of regular and irregular modes of the process of heat treatment of capillary-porous materials. Using this scheme makes it possible to take into account the effects of *memory*

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and self-organization of material. Initially, studies have been carried out to find an effective method for identifying fractal parameters of models [1, 7].

Replacing real environment properties with their idealized models is based on the fact that some of the properties appear most clearly. Then, by removing some irrelevant factors, the ideal model can be constructed. It can be characterized by these dominant 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 series or parallel connection of the elastic element, behavior of which obeys the Hooke's law, and the viscous one, obeys the Newton's law of viscosity [12, 16].

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 typical for a wood [8]. Therefore, it is suggested to use the fractional-order integro-differentiation mathematical apparatus to record the Newton's law of viscosity. It allows us to take into account the above mentioned properties of material.

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 capillary-porous materials taking into account the effect of *memory* and self-organization in the heat treatment process to provide appropriate quality of the material.

The algorithm for the 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 wood creep was approximated using fractional exponential operators also identified relationship between the fractional component and materials species, temperature and humidity fields.

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

10.2. DEFINITION OF THE PROBLEM

10.2.1. THE VISCOELASTIC DEFORMATION PROBLEM

The mathematical model of the rheological behavior of anisotropic capillary-porous materials in the heat treatment process taking into account the fractal structure of the environment can be described by equations of equilibrium with fractional order γ $(0 < \gamma \leq 1)$ in spatial coordinates x_1 and x_2 for the sample with such spatial dimensions $\Omega = \{x_1; x_2\} = \{[0; l_1] \times [0; l_2]\}$ [11-15]

$$C_{11}\left(\frac{\partial^\gamma \varepsilon_{11}}{\partial x_1^\gamma}(1-\bar{R}_{11})-\frac{\partial^\gamma \varepsilon_{T1}}{\partial x_1^\gamma}+\tilde{R}_{11}\right)+C_{12}\left(\frac{\partial^\gamma \varepsilon_{22}}{\partial x_1^\gamma}(1-\bar{R}_{12})-\frac{\partial^\gamma \varepsilon_{T2}}{\partial x_1^\gamma}+\tilde{R}_{12}\right)$$
$$+2C_{33}\left(\frac{\partial^\gamma \varepsilon_{12}}{\partial x_2^\gamma}(1-\bar{R}_{33}^2)-\frac{\partial^\gamma \varepsilon_{T3}}{\partial x_2^\gamma}+\tilde{R}_{33}^2\right)=0, \qquad (10.1)$$

$$C_{21}\left(\frac{\partial^\gamma \varepsilon_{11}}{\partial x_2^\gamma}(1-\bar{R}_{21})-\frac{\partial^\gamma \varepsilon_{T1}}{\partial x_2^\gamma}+\tilde{R}_{21}\right)+C_{22}\left(\frac{\partial^\gamma \varepsilon_{22}}{\partial x_2^\gamma}(1-\bar{R}_{22})-\frac{\partial^\gamma \varepsilon_{T2}}{\partial x_2^\gamma}+\tilde{R}_{22}\right)$$
$$+2C_{33}\left(\frac{\partial^\gamma \varepsilon_{12}}{\partial x_1^\gamma}(1-\bar{R}_{33}^1)-\frac{\partial^\gamma \varepsilon_{T3}}{\partial x_1^\gamma}+\tilde{R}_{33}^1\right)=0. \qquad (10.2)$$

The coefficients are defined as deformation vectors $\varepsilon^T=(\varepsilon_{11},\varepsilon_{22},\varepsilon_{12})$, $\varepsilon_T=(\varepsilon_{T1},\varepsilon_{T2},\varepsilon_{T3})^T$, vector components ε_T caused by changes in temperature ΔT and moisture content ΔU, assuming

$$\begin{gathered}\varepsilon_{T1}=\alpha_{11}\Delta T+\beta_{11}\Delta U,\\ \varepsilon_{T2}=\alpha_{22}\Delta T+\beta_{22}\Delta U,\\ \varepsilon_{T3}=0,\end{gathered} \qquad (10.3)$$

where $\alpha_{11},\alpha_{22},\beta_{11},\beta_{22}$ - coefficients of temperature expansion and humidity drying, $\overline{C}_{ij}$ - components of the elasticity tensor of the orthotropic body, $\bar{R}_{ij}$, $\tilde{R}_{ij}$ - value of integrals of relaxation kernels of fractional-differential models

$$\begin{gathered}\int_0^\tau R_{ij}(\tau-z,T,U)dz=\bar{R}_{ij},\\ \int_0^\tau R_{ij}(\tau-z,T,U)\frac{\partial^\gamma \varepsilon_{T1,T2}}{\partial x_k^\gamma}dz=\tilde{R}_{ij},\\ \int_0^\tau R_{ij}(\tau-z,T,U)\frac{\partial^\gamma \varepsilon_{T3}}{\partial x_2^\gamma}dz=\tilde{R}_{33}^2.\end{gathered} \qquad (10.4)$$

We set the following boundary and initial conditions

$$\begin{gathered}\varepsilon_{ij}\big|_{x_j=0}=0,\\ \varepsilon_{ij}\big|_{x_j=l_j}=0,\\ \varepsilon_{ij}\big|_{t=0}=0,(j=1,2).\end{gathered} \qquad (10.5)$$

Also the stress-deformable state of wood components should satisfy the equation of equilibrium.

10.2.2. THE HEAT-MASS TRANSFER PROBLEM

The mathematical model of the distribution of temperature-humidity fields in capillary-porous materials with a fractal structure, the stress-strain state of which is discussed in the paragraph 10.2.1, 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 [13, 14]

$$\begin{gathered} c\rho \frac{\partial^\alpha T}{\partial \tau^\alpha} = \lambda_1 \frac{\partial^2 T}{\partial x_1^2} + \lambda_2 \frac{\partial^2 T}{\partial x_2^2} + \varepsilon \rho_0 r \frac{\partial^\alpha U}{\partial \tau^\alpha}, \\ \frac{\partial^\alpha U}{\partial \tau^\alpha} = a_1 \frac{\partial^2 U}{\partial x_1^2} + a_2 \frac{\partial^2 U}{\partial x_2^2} + a_1 \delta \frac{\partial^2 T}{\partial x_1^2} + a_2 \delta \frac{\partial^2 T}{\partial x_2^2}. \end{gathered} \tag{10.6}$$

Those equations are solved using the appropriate initial conditions

$$\begin{gathered} T(\tau, x_1, x_2)|_{\tau=0} = T_0(x_1, x_2), \\ U(\tau, x_1, x_2)|_{\tau=0} = U_0(x_1, x_2). \end{gathered} \tag{10.7}$$

And boundary conditions of the third order

$$\begin{cases} \lambda_i \left. \frac{\partial T}{\partial n} \right|_{x_i = l_i} + \rho_0 (1 - \varepsilon) \beta \left(U|_{x_i = l_i} - U_P \right) = \alpha_i \left(T|_{x_i = l_i} - t_c \right), \\ a_i \delta \left. \frac{\partial T}{\partial n} \right|_{x_i = l_i} + a_i \left. \frac{\partial U}{\partial n} \right|_{x_i = l_i} = \beta \left(U_P - U_{x_i = l_i} \right), \end{cases} \tag{10.8}$$

$$\begin{cases} \lambda_i \left. \frac{\partial T}{\partial n} \right|_{x_i = 0} + \rho_0 (1 - \varepsilon) \beta \left(U|_{x_i = 0} - U_P \right) = 0, \\ a_i \delta \left. \frac{\partial T}{\partial n} \right|_{x_i = 0} + a_i \left. \frac{\partial U}{\partial n} \right|_{x_i = 0} = 0, \end{cases} \tag{10.9}$$

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, $\alpha_i(t_c, \nu)$ - heat transfer coefficient, $\beta(t_c, \phi, \nu)$ - moisture transfer coefficient, α - fractional order of derivative by the time ($0 < \alpha \leq 1$).

10.3. IDENTIFICATION OF FRACTIONAL-EXPONENTIAL CREEP KERNELS BY APROXIMATION THE EXPERIMENTAL DATA USING THE PRONI METHOD

The mathematical model (10.1)-(10.2) of viscoelastic deformation in fractal media for the one-dimension case can be written using the Boltzmann-Volterr’s integral equation [6]

$$\varepsilon(\tau) = \sigma_0 G(\tau) + \int_0^\tau \Pi(\tau - z, T, U) D_z^\alpha \sigma(z) dz, \tag{10.10}$$

$$\sigma(\tau) = \varepsilon_0 G'(\tau) + \int_0^\tau R(\tau - z, T, U) D_z^\beta \varepsilon(z) dz, \tag{10.11}$$

where $\alpha = \alpha(T, U)$, $\beta = \beta(T, U)$ fractional order of the derivative which are dependent on temperature T and moisture U; $\sigma(\tau)$ - tension; ε_0, σ_0 - the value of deformation and tension on the initial time τ_0; $G(\tau), G'(\tau)$ - time dependent functions; $\Pi(\tau - z, T, U)$, $R(\tau - z, T, U)$ - creep and relaxation kernels (memory functions), D_z^α, D_z^β - fractional derivatives by the variable z with the order α, β $(0 \leq \alpha, \beta \leq 1)$ respectively.

The general view of the creep kernel for fractional-differential rheological models (10.1)-(10.5) will be as follows [9]

$$\Pi(t) = \frac{1}{E\tau^\beta} t^{\beta - 1} E_{\psi_1, \psi_2}(\phi), \tag{10.12}$$

where E - modulus of elasticity, $E_{\psi_1, \psi_2}(\phi)$ - the Mittag-Leffler's function, $\tau = \eta E^{-1}$ (η -the coefficient of viscosity), $\psi_1 = \psi_1(\alpha, \beta)$, $\psi_2 = \psi_2(\alpha, \beta)$, $\phi = \phi(t, \alpha, \beta)$.

Since the Proni's approximation method, which is valid for a linear combination of exponential functions [2], will be used to parameters identification of creep data, the equation (10.11) will be transformed.

The two-parameter Mittag-Leffler's function is given by the formula [18]

$$E_{\alpha,\beta}(\tau) = \sum_{j=0}^{\infty} \frac{\tau^j}{\Gamma(\alpha j + \beta)}. \tag{10.13}$$

Taking into account equation (10.12) and the corresponding substitutions, we rewrite the appearance of the creep kernel (10.11) as follows

$$\Pi(s) = \sum_{i=0}^{n} A_i e^{-\lambda_i s}, \tag{10.14}$$

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

In [4], 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

$$\sum_{i=0}^{n} c_i \Pi(s + ih) = 0, \tag{10.15}$$

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

Since (10.13) is a solution of equation (10.14), then parameters λ_i can be found by using this method [2]. Let $e^{-\lambda_i h} = \xi_i$ then to determine each value ξ_i we need to solve the algebraic equation

$$c_0 + \sum_{i=1}^{n} c_i \xi^i = 0. \tag{10.16}$$

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

$$\begin{cases} \Pi_1^* c_0 + \Pi_2^* c_1 + \ldots + \Pi_n^* c_{n-1} + \Pi_{n+1}^* = 0, \\ \Pi_2^* c_0 + \Pi_3^* c_1 + \ldots + \Pi_{n+1}^* c_{n-1} + \Pi_{n+2}^* = 0, \\ \ldots \\ \Pi_n^* c_0 + \Pi_{n+1}^* c_1 + \ldots + \Pi_{2n-1}^* c_{n-1} + \Pi_{2n}^* = 0, \end{cases} \tag{10.17}$$

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

Finding from (10.14) the *n* solutions $\xi = \xi_1, \xi_2, \ldots, \xi_n$ we can find the parameters λ_i

$$\lambda_i = -\frac{\ln \xi_i}{h}. \tag{10.18}$$

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

$$\begin{cases} A_1^{'} + A_2^{'} + \ldots + A_m^{'} = \Pi_1^*, \\ A_1^{'} p_1 + A_2^{'} p_2 + \ldots + A_m^{'} p_m = \Pi_2^*, \\ \ldots \\ A_1^{'} p_1^{n-1} + A_2^{'} p_2^{n-1} + \ldots + A_m^{'} p_n^{n-1} = \Pi_n^*, \end{cases} \tag{10.19}$$

where $p_i = e^{-\lambda_i h}$, $A_i^{'} = \frac{A_i e^{-\lambda_i s_0}}{\lambda_i}$, $i = \overline{1, n}$, $s_0 = \ln \tau_0$ - initial moment.

The fractionally-exponential creep kernels can be identified according to the following experimental data [17], which are given in Table 10.1.

Table 10.1. 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 sufficient to distinguish two exponential functions for each rheological model. Accordingly, the 2^n ordinates are required to find λ_i parameters. To do this, let us divide the experimental data into 4 groups by summing up six ordinates in each. As a result, we get $\Pi_1^* = 15.28$, $\Pi_2^* = 17.28$, $\Pi_3^* = 9.49$, $\Pi_4^* = 4.88$. The system of linear equations (16) will bring the form

$$\begin{cases} 15.28 c_0 + 17.28 c_1 + 9.49 = 0, \\ 17.28 c_0 + 9.49 c_1 + 4.88 = 0. \end{cases} \tag{10.20}$$

That gives, $c_0 = 0.0373$, $c_1 = -0.5822$. The algebraic equation (10.15) will have the form

$$\xi^2 - 0.5822\xi + 0.0373 = 0, \tag{10.21}$$

the roots are respectively equal $\xi_1 = 0.5089$, $\xi_2 = 0.0733$.

The initial time moment according to our experimental data is $\tau_0 = 10^3$ h and step $\Delta t = 500$ h. Taking into account the corresponding replacement of variables, the h value in formula (10.18) will be equal to 37.29. The values of λ_i will be as follows: $\lambda_1 = 0.0181, \lambda_2 = 0.0701$.

Here are the obtained creep kernels for the Maxwell's, Voigt's and Kelvin's fractional-differential models [9]

$$\Pi_M(\tau) = \frac{1}{E\tau_{rel}^{\beta}}\left(\frac{\tau^{\beta-1}}{\Gamma(\beta)} + \frac{\tau_{rel}^{\alpha}\tau^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}\right), \qquad 0 \le \alpha < \beta \le 1, \tag{10.22}$$

$$\Pi_F(\tau) = \frac{1}{E\tau_{rel}^{\beta}}\tau^{\beta-1}E_{\beta-\alpha,\beta}\left(-\frac{\tau^{\beta-\alpha}}{\tau_{rel}^{\beta-\alpha}}\right), \qquad 0 \le \alpha < \beta \le 1, \tag{10.23}$$

$$\Pi_K(\tau) = \frac{\tau^{\beta-1}}{E\tau_{rel}^{\beta}}E_{\beta,\beta}\left(-\frac{\tau^{\beta-\alpha}}{\tau_{rel}^{\beta-\alpha}}\right), \qquad 0 \le \alpha \le 1;\ 0 < \beta \le 1, \tag{10.24}$$

where τ_{rel} – relaxation time.

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 the fractional-differential parameters as $\alpha = 0.0520$, $\beta = 0.9819$.

Using formula (10.12), we find parameters λ_1 and λ_2 for the Voigt and Kelvin models, which will have the following form: $\lambda_1 = 1 + \alpha - 2\beta$, $\lambda_2 = 1 - \beta$. 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 $E = 13800$ MPa.

In the expressions describing the creep kernels, the parameter $\tau = \eta E^{-1}$ is still unknown. We can determine it by finding the amplitudes A_i. To do this, we must solve the system of linear equations (10.18)

$$\begin{cases} A_1' + A_2' = 15.28, \\ A_1'p_1 + A_2'p_2 = 9.49. \end{cases} \tag{10.25}$$

Since λ_i and h are known, then $p_1 = e^{-0.6749}$, $p_2 = e^{-2.6139}$. 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 is not in the range of amplitude values, we find the τ parameter from equation $A_1 = \tau^{-\beta}/(E\Gamma(\beta))$. For Maxwell and Voigt models the parameter $\tau_{M,F} = 0.155 \cdot 10^{-3}$, for Kelvin is $\tau_K = 0.975 \cdot 10^{-2}$.

10.4. RESULTS OF SIMULATIONS

10.4.1. IDENTAFICATION OF PARAMETERS

For the sample of pine wood, whose modulus of elasticity is $E = 13{,}8$ MPa 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 (10.12) were identified from the experimental wood creep data [10, 17] for the Voigt model (Fig. 10.1), as well as for the Maxwell and Kelvin models. They were investigated under constant load and in the absence thereof.

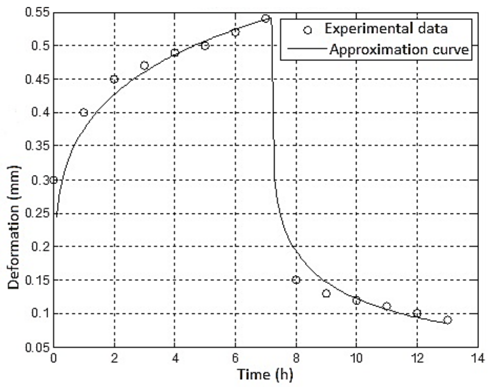

Fig. 10.1. Identification of fractional-differential parameters for the Voigt model at wood humidity W=7.5 %

The obtained functions of deformations depending on time are similar to the well-known model of hygro (thermo)-mechanical deformations which describe the processes in wood when the load, temperature and humidity are changed. The developed model also takes into account the formation of residual deformations which are characterized by the *memory* effects of wood. According to Fig. 10.1 after unloading of the material, the creep deformities remain. The maximum deviation of the approximate values from the experimental ones does not exceed 6.7%. It can be concluded that approximation in the form of a linear combination of Mittag-Leffler's functions is an effective tool for extrapolation of the experimental creep data of wood.

After analyzing the data from Fig. 10.2 and Fig. 10.3, the dependence between the identified fractional parameter α and the initial temperature, moisture content and wood species was established. For materials with higher density, it deviates slightly from the value $\alpha = 1$. It means, these parameters have small influence on the fractional properties of those materials. When the initial temperature or humidity, are lower these properties are more pronounced.

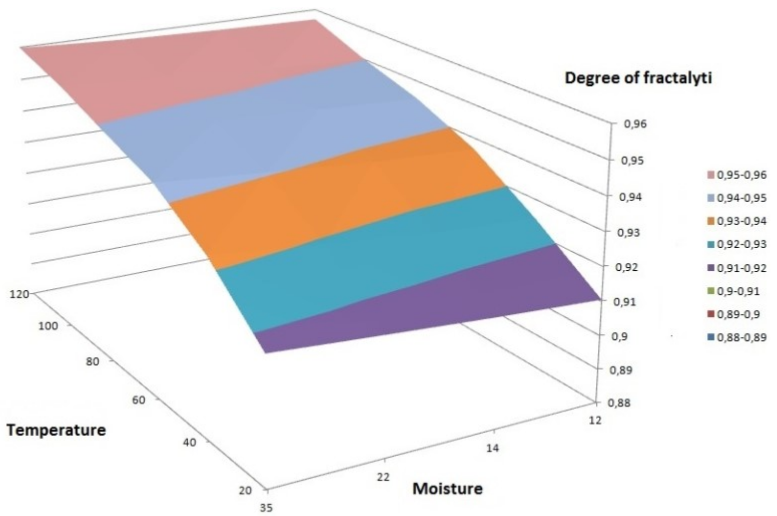

Fig. 10.2. Fractional parameter α for oak depending on temperature and humidity

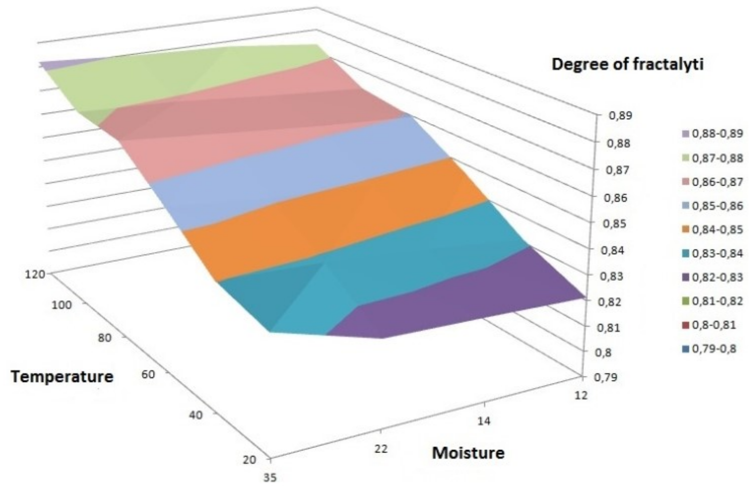

Fig. 10.3. Fractional parameter α for pine depending on temperature and humidity

Thus, the experimental data of wood creep are approximated using fractional-exponential functions and their fractional parameters are distinguished. They describe the influence of the fractal structure of the material. The coefficients of creep and relaxation kernels which are necessary for implementation of the mathematical model of heat-mass transfer (10.6)-(10.9) and viscoelastic deformation (10.1)-(10.5) of capillary-porous materials with fractal structure are obtained.

10.4.2. THE VISCOELASTIC DEFORMATION

Let us carry out the numerical implementation of the mathematical model (10.1)-(10.5) of viscoelastic 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 [9, 12, 14, 15] is used to find the numerical solution of the two-dimensional viscoelastic deformation problem. The dynamics of the stress components σ_{12} for different wood species depending on change of fractal items is shown as an example.

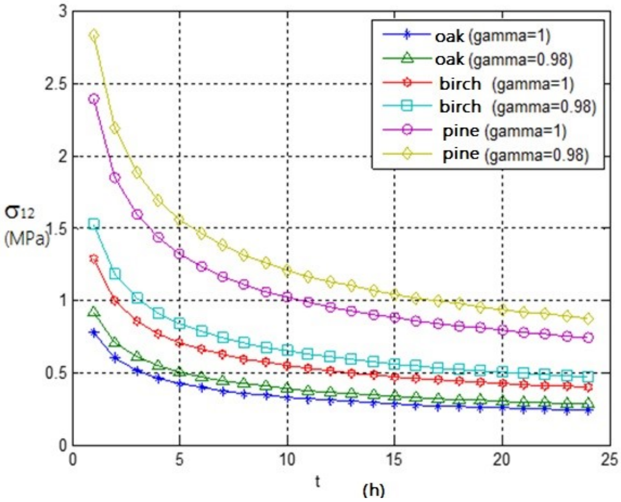

Fig. 10.4. Dynamic of the stress components σ_{12}

The influence of fractal parameters on the dynamics of stresses and strains components is analyzed (Fig. 10.4). It is determined that the difference between the stress components assuming fractal and monolithic structures does not exceed 16.7% for wood with higher density, but for the wood with lower density it reaches 19.6 - 24%.

10.5. CONCLUSIONS

Taking into account the two-parameter Mittag-Leffler's function and the corresponding substitutions, the general form of the original problem is reduced to the linear combination of exponential functions. After the transformations, the Proni's method can be applied. Fractional-differential parameters for Maxwell, Kelvin, and Voigt models of viscous-elastic deformation are identified. The properties of fractional models of viscoelastic deformation in fractal media are taken into account. As we presented, some other conditions must be fulfilled in order to apply the Proni's method described above.

The obtained results can be used for further investigation of mathematical models of viscoelastic deformation and heat transfer processes in fractal media.

For the fractional Voigt model for hardwood, 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 capillary-porous material during drying, it is possible to record the formation of residual deformations, the magnitude of which is defined as the difference between the viscoelastic deformations in the initial state (heated or wet wood) and the end state (chilled or dry wood). Residual stresses describe the memory effect of wood during drying.

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