Mathematical Modeling of Deformation-Relaxation Processes under Phase Transition

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Abstract: **This paper presents the mathematical modeling of deformation-relaxation processes under phase transition.**

Keywords: **phase transition, capillary-porous materials, viscoelastic stresses, deformation-relaxation processes, heat-mass-exchange processes.**

I. Introduction

During the process of drying capillary-porous materials, the zone of evaporation of moisture is deepening to the middle of the material. The presence of moving boundary of phase transformations at the interface between phases with different thermophysical and mechanical characteristics considerably complicates the mathematical models of deformation-relaxation and heat-mass-exchange processes during the drying of capillary-porous materials The modeling of heat-mass-exchange process with phase transitions in the drying process is diminished to the solving of Stefan's problem, which is the most complicated even for minor changes of material's density in the evaporation zone. However, the evaporation of water causes a change of its volume of almost a thousand times, and the removal of the vapor-gas mixture from the evaporation zone requires significant energy expenditures. With the deepening of the evaporation zone in the volume of the drying material, appears a significant increase of a pressure near the evaporation front. Therefore, taking into account the energy consumption of the steam movement kinetics and the convective heat transfer to the evaporation zones is included into different approaches of representing the evaporation zone model. If the material being drying is characterized by rheological properties, the part of energy associated with irreversible deformations is dissipated in the material. Therefore, the equation of the balance of dysplasia energy on the surface of the phase transition makes it possible to formulate conditions for the zone of deepening of the evaporation, taking into account the storage of irreversible deformations at phase transitions.

The development of mathematical models of viscoelastic capillary-porous materials in the process of drying is based on models of consequential creep [1,2]. However, such models describe the rheological behavior of different environments for a continuous history of deformation. In case the process of deformation of capillary-porous environments has implicit phase transitions and on their boundaries it is characterized by ruptures, it is necessary to take into account the influence of the previous history of the load on the phase transition on the further development of the stress-deformed state of the environment. For homogeneous viscoelastic environments that have changed the phase transition during deformation process, a hypothesis is used to preserve viscoelastic stresses at the transition boundary [3].This hypothesis is based on the using the main theorems of the theory of viscoelasticity, in particular Ries's theorem, in case the deformations of the environment are characterized by ruptures.

In this paper, this hypothesis is generalized in the case of viscoelastic deformation of anisotropic capillary-porous materials under conditions of temperature-humidity loading, taking into account the phase transition at the boundary of the zone of moisture evaporation. In particular, in the damp zone of the drying process, wood is considered as an orthotropic unsaturated polyphase capillary-porous material with taking into account viscoelastic properties, and in the dry zone, the deformation process is described by the equation of linear viscoelasticity with taking into account the orthotropy of the thermo-mechanical characteristics and the drying up of the material.

II. Statement of the Problem and the Results of The Study

For modeling the rheological behavior of colloidal capillary-porous materials, in particular wood, a model of a heterogeneous system with double porosity for a saturated system is used. Wood is considered as a three-phase system, which consists of wood material (solid phase), liquid and steam- air phases [4]. The distinction of this approach is that the wood is characterized by viscoelastic properties and explicitly describes the volumetric contents of each phase.

Deformation-relaxation processes are described by the following relations:

$$\varepsilon_{ij} = K^{s}_{ijke}\Big(\sigma_{ke} + \overline{\alpha}_{12}\delta_{ke} + \int_0^{\tau} K^{s}_{ijke}(\tau-\tau')\cdot (\sigma_{ij} + \overline{\alpha}_{12}\delta_{ke})d\tau'\Big) + + K^{f}_{ijke}\Big(\sigma_{ke} + \overline{\beta}_{12}\delta_{ke} + \int_0^{\tau} K^{f}_{ijke}(\tau-\tau')\cdot\big(\sigma_{ke} + \overline{\beta}_{12}\delta_{ke}\big)d\tau'\Big) + \alpha^{s}_{ij}\big(\Delta U(\tau)\big), \quad (1)$$

where $\varepsilon_{ij}, \sigma_{ij}$ – components of deformations and stresses, $K^{s}_{ijke} = K^{s}_{ijke}(0)/\alpha_3$; $K^{f}_{ijke} = K^{f}_{ijke}(0)/(1-m_{\Pi})$; $\overline{\alpha}_{12} = \alpha_1 p_1 + \alpha_2 p_2$; $\overline{\beta}_{12} = \beta_1 p_1 + \beta_2 p_2$; $\beta_i = m_{\Pi}\alpha_{ni} + \alpha_{ki}(1-m_{\Pi})$; $\alpha_i = \alpha_{ni} m_{\Pi} + \alpha_{ki} m_k$,

$(i=1,2)$; $\alpha_{n1}+\alpha_{n2}=1$; $\alpha_{k1}+\alpha_{k2}=1$; $K_{ijke}(0)$ - tensor of instantaneous sensibility, Пa^{-1}; β_{ij} - coefficient of moist expansion; $K_{ijke}(\tau-\tau')$ – tensor of creep velocity functions; $\Delta U(\tau)=U(\tau,x)-U_0(\tau)$ – the difference between the current humidity of the wood and its initial value; *p* – pressure; τ – time; m_{Π} – porosity, which is determined by the ratio of the volume of macropore to the volume of the material; m_k – porosity, which is determined by the ratio of volume of capillaries to the volume of cell walls; $\alpha_{ni,}\ \alpha_{ki}\ (i=1,2)$ – the contents of the liquid and vapor phases in the volume of pores and capillaries accordingly; the indices *f* refer to the effective values (woody skeleton); *S* – to the material of wood material; *П* – to the macropore system; *k* – to the system of capillaries; $\alpha_1,\alpha_2,\alpha_3$ – volumetric contents of steam-air, liquid and solid phases; δ_{ke} – unit tensor.

In the dried area, the rheological behavior of wood is described by linear equations of viscoelasticity with consideration of drying up. They include equilibrium equations $\partial\sigma_{ij}/\partial x_{ij}=0$ and linear integral equations of consequence creep for anisotropic environment.

$$\varepsilon_{ij}(\tau)=\beta_{ij}\left(\Delta U(\tau)+\int_0^{\tau}K^{s}_{ijke}(\tau-\tau')d\sigma_{ke}(\tau)\right) \tag{2}$$

Generally, the hypothesis of preserving the residual stresses in the wood as a capillary-porous viscoelastic environment for the phase transition in the case when the material in the damp state during drying process is a polyphase viscoelastic environment, and in the dry state, the wood is described by the equation of consequential creep.

Consider that at the time point $\tau=\tau^*$ and at the point $x=\xi(\tau^*)$, there is a transition from one zone to another. For $0<\tau<\tau^*$ the relation between tensions and deformations with material drying up taken into account is rarely (2) described by the equations

$$\sigma^{(1)}_{зал}(\tau^*)=-\int_0^{\tau^*}R^{з(1)}_{ijke}(\tau^*-\tau')\varepsilon^{(1)}_{ij}d(\tau')- \\ -\beta^{(1)}_{ij}\Delta(U(\tau')). \tag{3}$$

For the unsaturated wet region, the stress-strain state of wood, taking into account (1), is described by the relations

$$\sigma^{(2)}_{ij}(\tau)=R^{(2)s}_{ijke}\Big(\varepsilon^{(2)}_{ke}+\tilde{\alpha}_{12}\delta_{ke}+\int_0^{\tau}R^{(2)s}_{ijke}(\tau-\tau')\cdot \\ \cdot\left(\varepsilon^{(2)}_{ij}+\tilde{\alpha}_{12}\delta_{ke}\right)d\tau'\Big)+R^{(2)f}_{ijke}\Big(\varepsilon^{(2)}_{ke}+\tilde{\beta}_{12}\delta_{ke}+ \\ +\int_0^{\tau}R^{(2)f}_{ijke}(\tau-\tau')\cdot\left(\varepsilon^{(2)}_{ij}+\tilde{\beta}_{12}\delta_{ij}\right)d\tau'\Big)+ \\ +\tilde{\alpha}^{(s)}_{ij}(\Delta U(\tau)), \tag{4}$$

where $R^{(2)}{}_{ijke}$ - components of the relaxation function tensor, which are determined by components of the creep tensor $K^{(s)}{}_{ijke}$; coefficients $\tilde{\alpha}_{12}$, $\tilde{\beta}_{12}$ and $\tilde{\alpha}^{(s)}_{ij}$ associated with the corresponding dependencies with $\overline{\alpha}_{12}$, $\overline{\beta}_{12}$ and $\alpha^{(s)}_{ij}$.

The components of viscoelastic stresses are obtained by eliminating instantaneous-elastic components. Taking into account that for the phase transition the values of the components of viscoelastic stresses remain the same, we find the components of the wood deformations, assuming that from the very beginning of deformation in the damp state and till the time point $\tau=\tau^*$ components of the viscoelastic tensions are equal:

$$\sigma^{(2)}_{ij}(\tau^*)=\int_0^{\tau^*}R^{(2)s}_{ijke}(\tau^*-\tau')\cdot\left(\varepsilon^{(2)}_{ij}+\tilde{\alpha}_{12}\delta_{ke}\right)d\tau'+ \\ +\int_0^{\tau^*}R^{(2)f}_{ijke}(\tau^*-\tau')\cdot\left(\varepsilon^{(2)}_{ij}+\tilde{\beta}_{12}\delta_{ij}\right)d\tau'+ \\ +\tilde{\alpha}^{(s)}_{ij}(\Delta U(\tau^*)). \tag{5}$$

The ratio is represented as follows:

$$\sigma^{(2)}_{ij}(\tau^*)=\int_0^{\tau^*}\left(R^{(2)s}_{ijke}(\tau^*-\tau')+R^{(2)f}_{ijke}(\tau^*-\tau')\right)\cdot \\ \cdot\varepsilon^{(2)}_{ij}d\tau'+\int_0^{\tau^*}R^{(2)s}_{ijke}(\tau^*-\tau')\cdot\tilde{\alpha}_{12}\delta_{ke}d\tau'+ \\ +\int_0^{\tau^*}R^{(2)f}_{ijke}(\tau^*-\tau')\cdot\tilde{\beta}_{12}\delta_{ij}d\tau'+\tilde{\alpha}^{(s)}_{ij}\Delta(U(\tau^*)). \tag{6}$$

Let's bring in the designation

$$\int_0^{\tau^*}R^{(2)s}_{ijke}(\tau^*-\tau')\cdot\tilde{\alpha}_{12}\delta_{ke}d\tau'=R_{\alpha}(\tau^*);$$

$$\int_0^{\tau^*}R^{(2)f}_{ijke}(\tau^*-\tau')\cdot\tilde{\beta}_{12}\delta_{ij}d\tau'=R_{\beta}(\tau^*).$$

Therefore, we receive

$$\sigma^{(2)}_{ij}(\tau^*)=\int_0^{\tau^*}R^{(2)s}_{ijke}(\tau^*-\tau')+R^{(2)f}_{ijke}(\tau^*-\tau')\cdot \\ \cdot\varepsilon^{(2)}_{ij}d\tau'+R_{\alpha}(\tau^*)+R_{\beta}(\tau^*)+\tilde{\alpha}^{(s)}_{ij}\Delta(U(\tau^*)). \tag{7}$$

Let's consider the ratio of the rheological behavior of wood as an unsaturated three-phase environment in the following form

$$\sigma^{(2)}_{ij}(\tau)=R^{(2)sf}_{ijke}+R^{(2)s}_{ijke}\overline{R}_{\alpha}(\tau')+R^{(2)f}_{ijke}\overline{R}_{\beta}(\tau')+ \\ +R^{(2)s}_{ijke}\int_0^{\tau}R^{(2)s}_{ijke}(\tau-\tau')\varepsilon^{(2)}_{ij}d\tau'+ \\ +R^{(2)f}_{ijke}\int_0^{\tau}R^{(2)f}_{ijke}(\tau-\tau')\varepsilon^{(2)}_{ij}d\tau'+\tilde{\alpha}^{(s)}_{ij}\Delta(U(\tau)), \tag{8}$$

where

$$\overline{R}_{\alpha}(\tau')=\int_0^{\tau} R_{ijke}^{(2)s}(\tau-\tau')\tilde{\alpha}_{ij}\delta_{ke}d\tau';$$

$$\overline{R}_{\beta}(\tau')=\int_0^{\tau} R_{ijke}^{(2)f}(\tau-\tau')\tilde{\beta}_{12}\delta_{ij}d\tau'.$$

Equating the integral expressions for the components of viscoelastic tensions, with (7) and (8) we receive

$$\varepsilon_{ij}^{(2)}=-\frac{R_{ijke}^{(2)s}(\tau^*-\tau')\varepsilon_{ij}^{(1)}(\tau')}{R_{ijke}^{(2)s}(\tau^*-\tau')+R_{ijke}^{(2)f}(\tau^*-\tau')}-$$
$$-\frac{R_{\alpha}(\tau^*)-R_{\beta}(\tau^*)-\beta_{ij}^{(1)}(\Delta U(\tau'))-\tilde{\alpha}_{ij}^{(s)}\Delta(U(\tau^*))}{R_{ijke}^{(2)s}(\tau^*-\tau')+R_{ijke}^{(2)f}(\tau^*-\tau')} \quad (9)$$

Taking into account that during the process of phase transition, components of viscoelastic stresses are retained, taking into account (4), (8), (9), we write down the defining relations for viscoelastic deformation of wood

$$\sigma_{ij}^{(2)}(\tau)=R_{ijke}^{(2)s}\left(\varepsilon_{ke}^{(2)}+\tilde{\alpha}_{12}\delta_{ke}\right)+R_{ijke}^{(2)f}\cdot$$
$$\cdot\left(\varepsilon_{ke}^{(2)}+\tilde{\beta}_{12}\delta_{ke}\right)+R_{ijke}^{(2)s}\int_0^{\tau}R_{ijke}^{(2)s}(\tau-\tau')\tilde{\alpha}_{12}\delta_{ke}d\tau'+$$
$$+R_{ij}^{(2)f}\int_0^{\tau}R_{ijke}^{(2)f}(\tau-\tau')\tilde{\beta}_{12}\delta_{ke}d\tau'+$$
$$+\int_0^{\tau^*}\frac{R_{ijke}^{(2)s}R_{ijke}^{(2)s}(\tau-\tau')+R_{ijke}^{(2)f}R_{ijke}^{(2)f}(\tau-\tau')}{R_{ijke}^{(2)s}(\tau^*-\tau')+R_{ijke}^{(2)f}(\tau^*-\tau')}\cdot$$
$$\cdot(R_{ijke}^{з(1)}(\tau^*-\tau')d\tau'-\tilde{\alpha}_{ij}^{(s)}\Delta(U(\tau^*)))d\tau'+ \quad (10)$$
$$+\left(R_{\alpha}(\tau^*)-R_{\beta}(\tau^*)-\beta_{ij}^{(1)}(\Delta U(\tau'))+\right.$$
$$+R_{ijke}^{(2)s}\int_{\tau^*}^{\tau}R_{ijke}^{(2)s}(\tau-\tau')\varepsilon_{ij}^{(2)}d\tau'+R_{ij}^{(2)f}\cdot$$
$$\cdot\int_{\tau^*}^{\tau}R_{ijke}^{(2)f}(\tau-\tau')\varepsilon_{ij}^{(2)}d\tau'+\tilde{\alpha}_{ij}^{(s)}\Delta(U(\tau)).$$

Thus, the obtained relations take into account the deformation-relaxation processes of the wood as a multiphase unsaturated environment for both before and after the evaporation zone of the moisture. In particular, the effect on stress relaxation in the wood of the prehistory of deformation to the phase transition is taken into account.

III. Results of the Numerical Experiment

The process of deformation of capillary-porous materials is characterized by a change of their volume. This causes a change of phase environment's size, which significantly impedes researching the rheological behavior of the material. Therefore, we consider the contribution of residual stresses to relaxation for a one-dimensional viscosity case taking into account the above-described phase transition. In this case, the functions of the rheological behavior of the wood taking into account the mechanism of accumulation of residual deformations [5,6] $K^{(s)}(\tau-\tau')$ and $K^{(f)}(\tau-\tau')$ we choose in the form

$$R^{(2)(i)}(\tau-\tau')=\left[a_0-\sum_{i=1}^{M}a_i\exp(-b_i\tau)\right]h(\tau)\cdot$$
$$\cdot h(\tau_0-\tau)-\left[a_0-\sum_{i=1}^{M}\alpha_i\exp(-\beta_i(\tau-\tau_0))\right]\cdot$$
$$\cdot h(\tau-\tau_0), \quad (11)$$

where $h(\tau)$ Heiviside's function, and the unknown coefficients $a_i, b_i, \alpha_i, \beta_i$ are determined by the method of least squares based on the approximation of experimental data on the creep of samples of timber under load and after unloading. In the general case, they are functions of temperature *T(x,τ)* and moisture *U(x,τ)*. To do this we use the method of minimum squares [7]. To quantify the difference, a statistical criterion was used based on the correlation coefficients [7].

To determine the parameters $\alpha_{i0}(i=1,2,3)$, taking into account the change in humidity, the correlation are obtained taking into account the conditions of additivity and the uniform distribution of phases over the wood regions. Then, in accordance with (9), (10), (11), (12) we obtain relations for determining the effect of residual stresses on wood during the phase transition for a one-dimensional deformation case

$$\Delta\sigma(\tau^*)=\int_0^{\tau^*}(\overline{E}\exp((\tau^*-\tau')/\tau_{рел}(U,T))\cdot$$
$$\cdot(\overline{R}_0^{(2)s}R^{(2)s}(\tau-\tau')+\overline{R}_0^{(2)f}R^{(2)f}(\tau-\tau')+$$
$$+\overline{R}^{(2)f}(\tau-\tau')))/(\overline{R}_0^{(2)s}R^{(2)s}(\tau^*-\tau')+$$
$$+\overline{R}_0^{(2)f}R^{(2)f}(\tau^*-\tau')+\overline{R}^{(2)f}(\tau^*-\tau'))\cdot \quad (12)$$
$$\cdot\varepsilon^{(1)}(\tau')d\tau',$$

where

$$\overline{R}_0^{(2)s}=R_0^{(2)s}(1-\varepsilon)\alpha_{20}\rho_2/\alpha_{30};$$
$$\overline{R}_0^{(2)f}=R_0^{(2)f}(1-\varepsilon)(\alpha_{30}+b(\alpha_{20});$$
$$\overline{R}^{(2)f}=\int_0^{\tau^*}R_0^{(2)f}R^{(2)f}(\tau^*-\tau')(\alpha_{30}+\alpha_{20})\cdot$$
$$\cdot\frac{\rho}{(\alpha_{30}+b\alpha_{20})}d\tau^*;$$
$$\alpha_{10}=1-\rho_W\left(\frac{1}{\rho_3}+\frac{U}{100\rho_1}\right)\cdot\frac{100}{100+U};$$
$$\alpha_{20}=\frac{1}{\rho_1-\rho_2}\left(\rho_W\left(\frac{1}{\rho_3}+\frac{U}{100\rho_2}\right)\cdot\right.$$
$$\left.\cdot\frac{100}{100+U}-\rho_1\right);$$

$$\alpha_{30} = \frac{1}{\rho_1 - \rho_2}\left(\rho_W\left(\rho_1 - \rho_3 - 1\right)\cdot\right.$$

$$\left.\cdot\left(1 + \frac{1}{\rho_3}\frac{U}{100\rho_2}\right)\cdot\frac{100}{100+U} - \rho_1\right);$$

$$\rho_W = \begin{cases} k_{\alpha 1}\rho_{12}\dfrac{100+U}{100+k_{\alpha 2}U}, U \le 30\%; \\ k_{\alpha 3}\rho_{12}\left(1+0{,}1U\right), U > 30\%, \end{cases}$$

where $k_{\alpha 1}, k_{\alpha 3}, \rho_{12}, b$ – coefficients determined by the properties of wood [5].

For the case of deformation changes at the moment of the phase transition, which are characterized by a change in density, depending on the change in humidity. Also, the linear dependence of modulus of elasticity on changes in humidity is taken.

The nature of the distribution of stress relaxation curves shows that the consideration of viscoelastic stresses during the phase transition in the wood during the drying process differs from stress relaxation curves without taking into account residual viscoelastic deformations.

In fig. 1 and 2 graphic dependences of relaxation of viscoelastic stresses in wood with a base density *ρ=530* kg/m^3 are given.

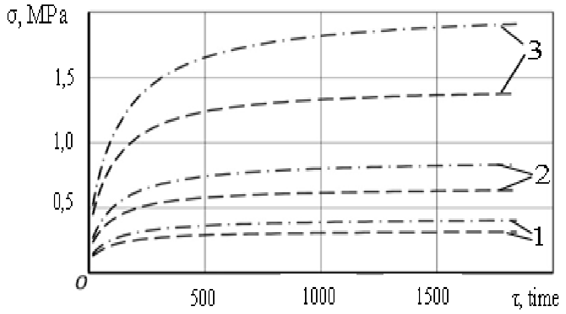

Fig.1 Dependencies of relaxation of stresses for materials of wood in the radial direction ρ_δ=550 (– · – · –), ρ_δ=400 (– – –) for different values of initial humidity (1–10%, 2–15%, 3–20%).

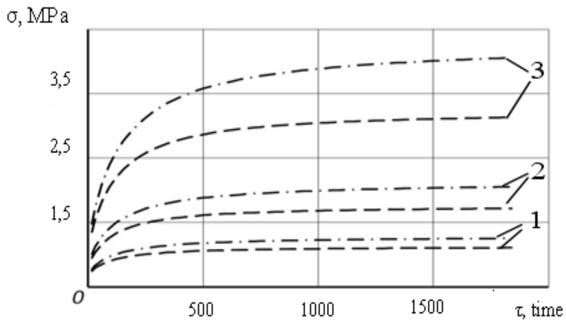

Fig.2 Dependencies of relaxation of stresses for materials of wood in the tangential direction ρ_δ=550 (– · – · –), ρ_δ=400 (– – –) for different values of initial humidity (1–10%, 2–15%, 3–20%).

IV. Conclusion

The mathematical model of determination of viscoelastic deformation of capillary-porous materials as a three-phase system with including anisotropy of thermo mechanical characteristics is given.

The regularities of the influence of transfer mechanisms on processes of viscoelastic deformation in the solid, liquid and vapor phases for wood are established.

Applied software for numerical implementation of mathematical models is developed.

A generalization of the hypothesis of the saving of irreversible deformations in the case of viscoelastic deformation of capillary-porous materials, taking into account the phase transition at the boundary of the evaporation of moisture is obtained.

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