Strength analysis of structures made of high-filled polymer materials: constitutive equations, methods of boundary value problems solving, account of strain concentration

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Abstract. We investigate strength, damage accumulation and failure of composite polymer materials with a high degree of dispersion filling (a few tens percent by volume). We consider the class of quasistatic loading processes with axial tension predominance, namely only one of the principal strains is positive (tensile) and its direction remains almost unchanged in the course of loading; hydrostatic pressure and temperature can be changed within certain limits.

On basis of the published experimental data derived under uniaxial uniform tension in various barothermal conditions (more than 50 non-stationary loading programmes) we suggest the equation system for modelling the mechanical behaviour of specified materials, namely: the deviatoric relation of gero-endochronic viscoelasticity, the quasielastic equation for volumetric deformation, the kinetic equations for damage and failure parameters, as well as the criterion of failure. The model has a hierarchical structure: first, the material functions are determined for active straining in the normal barothermal conditions; then, if necessary and if relevant experimental data are available, the material functions are determined for unloading and repeated loading, different values of hydrostatic pressure and temperature. The model identification procedure is relatively simple: the material functions are determined sequentially and each of them contains 1–3 constants.

The tensorial generalization of this equation system is proposed and the algorithm for numerical solving of initial-boundary value problems is described. This algorithm is implemented in ABAQUS software complex through the UMAT subroutine.

We carried out the finite-element analysis of short wide strips with and without holes or cuts in constant rate elongation processes. By comparison of simulation results with published experimental data it was established the need for taking into account the effect of stress-strain state concentration. For this purpose we propose the following generalization of the model: into the equations for damage and failure parameters we introduce the material function of the concentration parameter, which is the ratio of the definite state variable (namely, the failure parameter in the model without taking into account the concentration effect) at a current material point to the mean value of this variable in the point neighborhood of the definite radius. We specify the method for approximate reduction of initial-boundary value problem for the proposed nonlocal theory to the problem for piecewise homogeneous body, composed of a set of material layers, described by local constitutive equations. The method was successfully tested in the strength analysis of strips with holes and cuts (concentrators of middle and high level, respectively).

The obtained results show sufficient accuracy of the developed mathematical model – including adequate prediction of the moment and the location of a failure initiation.

Gero-endochronic viscoelastic constitutive model

In [1], the following equation system was proposed to describe the mechanical behaviour of high-filled polymer materials (HFPM):

$$S_\alpha(t)=\varphi\int_0^t R[t_*(t)-t_*(\tau)]d\text{Э}_\alpha(\tau)\,,\quad R(t)=\sum_{n=1}^{N}R_n\exp(-t/\tau_n)+R_\infty \tag{1}$$

$$\frac{dt_*}{dt}=\frac{\gamma(\omega)+[1-\gamma(\omega)]f(e_u,\xi,T)}{a_T(T)} \tag{2}$$

$$\frac{d\omega}{dt}=\begin{cases}e_u/[b_0g^{(d)}(e_u,\xi,T)], \text{ if } \ \chi=1\\ 0, \text{ if } \ \chi<1\end{cases}\,,\quad \omega(0)=0 \tag{3}$$

$$\frac{d\Omega}{dt}=\begin{cases}e_u/[b_0g(e_u,\xi,T)], \text{ if } \ \chi=1\\ 0, \text{ if } \ \chi<1\end{cases}\,,\quad \Omega(0)=0\,,\quad \Omega(t^{(F)})=1 \tag{4}$$

$$\varphi=\varphi(\omega,\xi,\chi) \tag{5}$$

$$\Theta=\psi(\omega,\xi,T)\sigma_u^* \tag{6}$$

Here σ_α and ε_α are the principal true stresses and the logarithmic strains ($\alpha=1,2,3$); $S_\alpha=\sigma_\alpha-\sigma$ and $\text{Э}_\alpha=\varepsilon_\alpha-\Theta/3$, $\sigma_u=(3S_\alpha S_\alpha/2)^{1/2}$ and $\varepsilon_u=(2\text{Э}_\alpha\text{Э}_\alpha/3)^{1/2}$, $3\sigma=\sum_\alpha\sigma_\alpha$ и $\Theta=\sum_\alpha\varepsilon_\alpha$ are their deviators, intensities and mean values, respectively; t_* is the reduced (internal) time; $\sigma_\alpha^*=\sigma_\alpha/\varphi$ is the reduced stresses; $e_u=(2\dot{\text{Э}}_\alpha\dot{\text{Э}}_\alpha/3)^{1/2}$ is the logarithmic strain rate intensity (the overdot denotes a time derivative); $a_T(T)$ is the temperature-time shift function; $\xi=\sigma/\sigma_u$ is the parameter of stress state form; $\chi=\varepsilon_u/\varepsilon_u^{(M)}$ is the strain activity parameter, $\varepsilon_u^{(M)}(t)=\max\limits_{\tau\in[0;t]}\varepsilon_u(\tau)$; ω and Ω are the damage and failure parameters (Ω is used only to determine the failure moment $t=t^{(F)}$). In [1], the model (1)-(6) was identified and verified on the basis of experimental data [2-4].

Constitutive equations in tensorial incremental form

Similar to [5], the equation system (1)-(6) is generalized to the following tensorial incremental form:

$$\begin{aligned}\boldsymbol{\sigma}(t+\Delta t)=\tilde{K}(t,\Delta t)\,[\ln J(t+\Delta t)-\tilde{\Theta}(t,\Delta t)]\,\mathbf{I}+\tilde{\varphi}(t,\Delta t)\mathbf{R}_t(t+\Delta t)\tilde{\mathbf{S}}(t,\Delta t_*)\mathbf{R}_t^{\mathrm{T}}(t+\Delta t)+\\ +\tilde{\varphi}(t,\Delta t)\tilde{R}(\Delta t_*)\left[\ln\mathbf{V}_t(t+\Delta t)-\mathrm{tr}\big(\ln\mathbf{V}_t(t+\Delta t)\big)\mathbf{I}/3\right]\end{aligned} \tag{7}$$

In this equation, $\boldsymbol{\sigma}(t+\Delta t)$ is the true stress tensor, $\mathbf{V}_t(t+\Delta t)$ is relative (with respect to configuration at the moment t) left stretch tensor, other variables and functions are:

$$\tilde{\mathbf{S}}(t,\Delta t_*)=\sum_{n=1}^{N+1}R_n\exp(-\Delta t_*/\tau_n)\,\mathbf{Э}^{(n)}(t)$$

$$\mathbf{Э}^{(n)}(t+\Delta t) = \exp(-\Delta t_* / \tau_n)\mathbf{R}_t(t+\Delta t)\mathbf{Э}^{(n)}(t)\mathbf{R}_t^{\mathrm{T}}(t+\Delta t)$$
$$+ F(\Delta t_* / \tau_n)\left[\ln \mathbf{V}_t(t+\Delta t) - \mathrm{tr}\big(\ln \mathbf{V}_t(t+\Delta t)\big)\mathbf{I}/3\right]$$

$$\tilde{\Theta}(t,\Delta t) = \ln J_T(t+\Delta t) + \left(\psi - \xi(t)\frac{\partial\psi}{\partial\xi}\right)\frac{\sigma_u(t)}{\tilde{\varphi}(t,\Delta t)}, \quad \tilde{\varphi}(t,\Delta t) = \varphi\big(\omega(t)+\Delta\omega, \xi(t), \chi(t)\big)$$

$$\tilde{K}(t,\Delta t) = \left[\frac{1}{K_0} + \frac{1}{\tilde{\varphi}(t,\Delta t)}\frac{\partial\psi\big(\omega(t)+\Delta\omega, \xi(t), T(t+\Delta t)\big)}{\partial\xi}\right]^{-1}$$

$$\tilde{R}(\Delta t_*) = \sum_{n=1}^{N+1} R_n F(\Delta t_* / \tau_n), \quad F(x) = \frac{1-\exp(-x)}{x}$$

$$\chi(t) = \frac{u\big(\boldsymbol{\varepsilon}(t)\big)}{\max\limits_{\tau\in[0;t]} u\big(\boldsymbol{\varepsilon}(\tau)\big)}, \quad e_u(t-\Delta t/2) = u\left(\frac{\ln \mathbf{V}_{t-\Delta t}(t)}{\Delta t}\right), \quad u(\mathbf{x}) = \sqrt{\frac{2}{3}\mathrm{tr}\big(\mathbf{x}^2\big) - \frac{2}{9}\left[\mathrm{tr}(\mathbf{x})\right]^2}$$

$$\boldsymbol{\varepsilon}(t+\Delta t) = \mathbf{R}_t(t+\Delta t)\boldsymbol{\varepsilon}(t)\mathbf{R}_t^{\mathrm{T}}(t+\Delta t) + \ln \mathbf{V}_t(t+\Delta t)$$

where $\boldsymbol{\varepsilon}(t)$ is the total strain tensor, $\mathbf{R}_t(t+\Delta t)$ is the relative (with respect to configuration at the moment t) rotation tensor at the moment $t+\Delta t$.

Numerical solution of three-dimensional initial-boundary value problems and comparison to experiment

In [6], the material Jacobian of constitutive equations (7) was obtained as :

$$[\delta_o \boldsymbol{\sigma}(t+\Delta t)]_{ij} = c_{ijpq}[\delta\boldsymbol{\varepsilon}]_{pq}, \quad c_{ijpq} = (\tilde{K} - \tilde{\varphi}\tilde{R}/3)\delta_{ij}\delta_{pq} + \tilde{\varphi}\tilde{R}(\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp})/2 \qquad (8)$$

The components of the material Jacobian (8) correspond to the linear elasticity tensor for a material with bulk modulus $\tilde{K}$ and shear modulus $\tilde{\varphi}\tilde{R}/2$.

Calculations of the true stress tensor (7) components and the material Jacobian (8) according to the given tensors $\ln \mathbf{V}_t(t+\Delta t)$, $\mathbf{R}_t(t+\Delta t)$ and the known scalar and tensorial state variables (at the beginning of actual time step) are implemented in the user subroutine UMAT (in the finite element package ABAQUS). Also, the state variables $e_u(t+\Delta t/2)$, $\chi(t+\Delta t)$, $\omega(t+\Delta t)$, $\Omega(t+\Delta t)$, $\mathbf{Э}^{(n)}(t+\Delta t)$ (at the end of actual time step) in this subroutine are calculated. Some examples of the strength analysis with use ABAQUS and the described UMAT are presented below.

In [7], the experimental data in constant cross-head rate tension processes of short wide strips (made of HFPM) with and without holes or cuts were published. We carried out the finite-element analysis of these processes in accordance with the model (7), (3), (4). “Load – global strain” dependence and failure moment for strips without holes and cuts is modelled quite adequate. But theoretical failure moment for strips with a hole or cut is much less then in fact. Therefore the model needs a generalization.

Method to take into account the effect of strain concentration

For this purpose, we propose to replace the material constant b_0 (in the kinetic equations (3) and (4) for damage and failure parameters) by the material function $\lambda(p_c)b_0$, where p_c is the parameter describing the strain concentration. Then the equations for ω and Ω obtain the following form:

$$\frac{d\omega}{dt}=\begin{cases} e_u/\left[b_0\lambda(p_c)g^{(d)}(e_u,\xi,T)\right], \text{ if } \chi=1 \\ 0, \text{ if } \chi<1 \end{cases}, \quad \omega(0)=0 \tag{9}$$

$$\frac{d\Omega}{dt}=\begin{cases} e_u/\left[b_0\lambda(p_c)g(e_u,\xi,T)\right], \text{ if } \chi=1 \\ 0, \text{ if } \chi<1 \end{cases}, \quad \Omega(0)=0, \quad \Omega(t^{(F)})=1 \tag{10}$$

Let us denote as Ω_0 the parameter calculated in formal accordance with the equations (4):

$$\frac{d\Omega_0}{dt}=\begin{cases} e_u/\left[b_0 g(e_u,\xi,T)\right], \text{ if } \chi=1 \\ 0, \text{ if } \chi<1 \end{cases}, \quad \Omega_0(0)=0 \tag{11}$$

The field Ω_0 is used to define the parameter p_c:

$$p_c(t,\mathbf{x})=\Omega_0(t,\mathbf{x})/\Omega_0^{(R_c)}(t,\mathbf{x}), \quad \Omega_0^{(R_c)}(t,\mathbf{x})\equiv \int\limits_{|\mathbf{x}'-\mathbf{x}|\le R_c}\Omega_0(t,\mathbf{x}')d\mathbf{x}' \Big/ \int\limits_{|\mathbf{x}'-\mathbf{x}|\le R_c} d\mathbf{x}' \tag{12}$$

i.e. $p_c(t,\mathbf{x})$ is the ratio of the local (at the material point $\mathbf{x}$) value of Ω_0 to the mean value of Ω_0 in the R_c-neighbourhood (of this point $\mathbf{x}$); the time t is a parameter in this definition. In the case of uniform strain process, it is evidently $p_c(t,\mathbf{x})\equiv 1$, therefore $\lambda(1)=1$. The parameters Ω_0 (11) and Ω (10) coincide, if $\lambda(p_c)\equiv 1$.

The solving of initial-boundary value problem using the model (7), (9)-(12) is carried out by two phases. First, the preliminary numerical strength analysis of the body is performed with the assumption $\lambda(p_c)=1$, i.e. using the model (7), (3), (4); this analysis ends at some moment $t=t_A^{(F)}$, when at some point A of the considered body V the parameter Ω_0 reaches 1 for the first time. Then the "hand-made" preparation for the basic strength analysis is followed. Using the obtained field $\Omega_0(t_A^{(F)},\mathbf{x})$, the domains $V^{(i)}\subset V$ with $p_c>1.1$ (for 10% level of error tolerance) are determined. It is supposed that in the rest of V the strain concentration is insignificant (if $p_c\in(1;1.1]$) or does not affect the material behaviour (if $p_c\in[0;1]$). In each domain $V^{(i)}$ the point $A^{(i)}$ with maximal value of the parameter p_c is determined. The values of p_c at a several points in a several directions starting from the point $A^{(i)}$ are calculated using ABAQUS resource. These data make it possible to build the isolines and then the isosurfaces with $p_c(\mathbf{x})=p_c^{(i)(j)}=\text{const}$, $j=0,1,\dots,N^{(i)}$, where $p_c^{(i)(j)}\in[1.1;\,p_c(A^{(i)})]$, $p_c^{(i)(0)}=1.1$, $p_c^{(i)(N^{(i)})}=p_c(A^{(i)})$. Thus, each domain $V^{(i)}$ is divided into the layers $V^{(i)(j)}$, $j=1,\dots,N^{(i)}$. Within $V^{(i)(j)}$ it is supposed that

$p_c(\mathbf{x}) = p_c^{(i)(j)} = \text{const}$, therefore $\lambda(p_c) = \lambda(p_c^{(i)(j)})$ in the equations (9), (10). That enables to specify all mechanical properties in each layer ("partition" in the ABAQUS terminology) $V^{(i)(j)}$.

The final strength analysis is executed for the piecewise homogeneous body V, composed of the material layers $V^{(i)(j)}$ and the rest of V, where it is supposed $\lambda(p_c) = 1$. This analysis is in essence the approximate solution of original initial-boundary value problem for the nonlocal model (7), (9)-(12), in which the material properties at a current material point depend not only on strain history at this point but also on values of Ω_0 in the point neighbourhood of the definite radius R_c.

The material function $\lambda(p_c)$ and the material constant R_c are determined on the basis of experimental data at the moment of local failure of specimens in which a different strain concentration levels are realized. Such tests are included in the list of basic tests used for identification of the model (7), (9)-(12). The values of R_c and $\lambda(p_c)$ are chosen under condition that the moment of local failure in the initial-boundary value problem solution corresponds to the test. The identified R_c and $\lambda(p_c)$, and also the values of $N^{(i)}$, $p_c^{(i)(j)}$, suitable for a different strain concentration levels, are used for the strength analysis of other bodies made of this material.

Now we demonstrate some results of the strength analysis of the tests [7]. Owing to their symmetry it is reasonable to consider a quarter of each strip. Fig. 1 concerns a strip 25.4 mm long with a central hole 12.7 mm diameter and shows location and configuration of the layers $V^{(1)(j)}$ composing the only domain $V^{(1)}$ wherein a significant strain concentration takes place; at that $j = 1,...,N^{(1)}$, $N^{(1)} = 5$, $p_c^{(1)(1)} = 1.15$, after intermediate value $p_c^{(1)(2)}$ the differences $(p_c^{(1)(j+1)} - p_c^{(1)(j)})$ are accepted the same for all $j = 2,...,N^{(1)} - 1$, and in the end $p_c^{(1)(N^{(1)})} = p_c(A^{(1)}) = 1.5$. Fig. 2 is the same for a strip with a central cut if the cut tip is modelled by the rounding with radius $r = 0.25$ mm (this value of r is the upper bound estimate of the size of filler particles in the considered material); at that $N^{(1)} = 10$, $p_c^{(1)(1)} = 1.4$, $p_c(A^{(1)}) = 10.0$. The strength analysis for the cases $r = 0.5$, 1 [mm] was done also (see [6]).

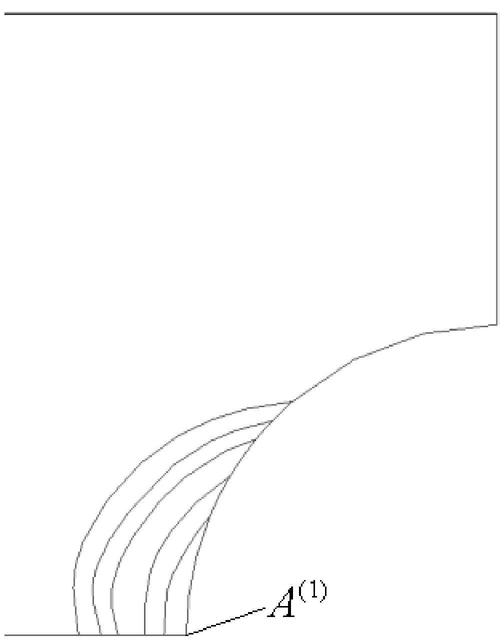

Fig. 1. The layers $V^{(1)(j)}$ in a strip with a hole.

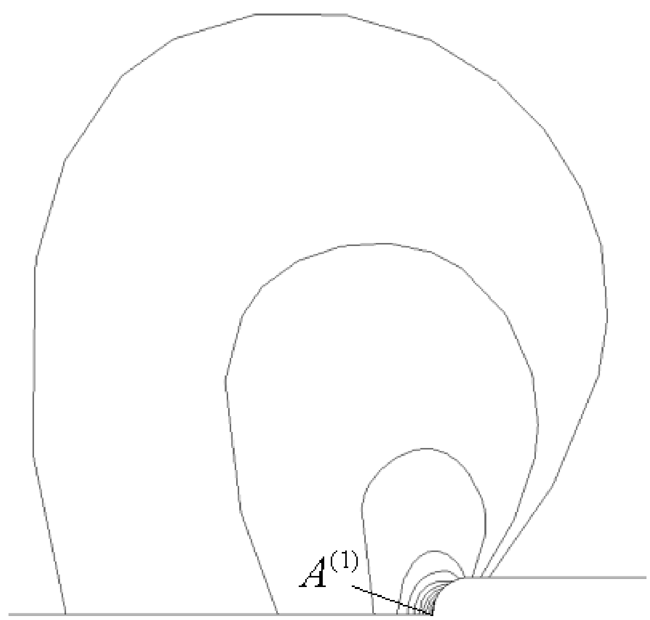

Fig. 2. The layers $V^{(1)(j)}$ in a strip with a cut.

The value $R_c = 5$ mm was chosen. The function $\lambda(p_c)$ was approximated in the following form:

$$\lambda(p_c) = 1 + \min\{[M(p_c - 1)/a_c]^{n_c};\ M(p_c - 1)\} \qquad (13)$$

where $M(x) \equiv xH(x)$, $H(x)$ is the Heaviside function. The material constants $a_c = 1.6$, $n_c = 0.685$ were determined under condition that the theoretical value of "global strain" at the moment of local failure corresponds to the experimental value for strip with a hole and strip with a cut (approximate 0.1 и 0.06 respectively, as it was measured in [7]). For more details of the determination of R_c, $\lambda(p_c)$, $N^{(i)}$, $p_c^{(i)(j)}$ see [6].

Fig. 3 shows some results of the strength analysis using the model (7), (9)-(12) with the function $\lambda(p_c)$ (13) and the specified a_c, n_c, R_c, $N^{(1)}$, $p_c^{(1)(j)}$. The theoretical lines with the first symbol *0*, *1*, *2* concern strips without a defect, with a hole, with a cut, respectively. The second symbol *c* indicates the solution with taking into account the effect of strain concentration (using the model (7), (9)-(12)), in contrast to the using the model (7), (3), (4) solution, which is indicated by second symbol *n*. The oblique cross on each theoretical line indicates the start of a local failure (the parameter Ω reaches 1 for the first time). Global stress $\Sigma(t)$ is defined as $F(t)/S_{\min}(0)$, where $F(t)$ is a current value of applied tensile load, $S_{\min}(0)$ is the initial area of the minimal cross-section of specimen. Global strain E is $L(t)/L(0)-1$, where $L(t)$ is a current value of the specimen length. Experimental data [7] are marked by square, round, triangular symbols for strips without a defect, with a hole, with a cut, respectively. In all tests presented in fig. 3, the strips were identical except a defect, the global strain rate $\dot{E}$ was the same (0.1 min^{-1}). Fig. 3 demonstrates a sufficiently correct simulation of strength and failure beginning in these significant model tasks. In [6], the strength analysis for the rest of the tests [7] (defect-free strips of different cross-section under straining with different values of $\dot{E}$) was done also.

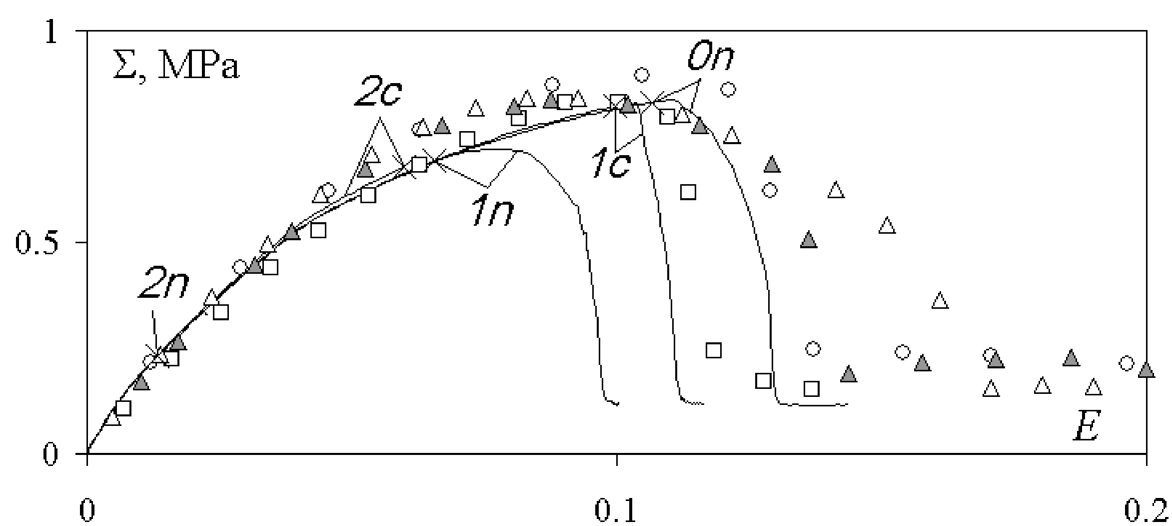

Fig. 3. "Global stress – global strain" dependencies for strips without a defect, with a hole, with a cut.

Summary
The problem of the constitutive model for the high-filled polymer materials under predominant axial tension (including the barothermal effects) was considered. The complete mechanical and mathematical apparatus for the strength analysis was developed, namely:
1) constitutive equation system (with the failure criterion) including nonlocal effects of strain concentration;
2) practicable procedure (with the list of basic tests) for model identification and results of model verification in extensive set of relevant experimental data;
3) user subroutine for material properties modelling in the finite element package for numerical solving of initial-boundary value problems;
4) adaptation of standard numerical stress analysis procedure to the case of nonlocal model of damage accumulation and failure.

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