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GENERALIZED MODEL OF VISCOELASTIC DEFORMATION

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Abstract: In this paper we consider generalized mathematical model describing the process of viscoelastic deformation of polymer materials. It describes the polyethylene creep under diffusion of liquid environment not interacting chemically with the polymer. We analyse here some results of certain tests produced with samples which have reached beforehand different levels of saturation with cyclohexan and have been afterwards put under mechanical testing of a short creep in pure torsion and uniform loading. Analyzing the results we use the method of orthogonal expansions and at the same time extend it for a process with integrating properties (without self-settling). In this case it is necessary to separate the integral component, which is presented as signal-dependent.

1. Introduction

In this paper we investigate a generalized model describing the process of viscoelastic deformation of polymer materials which are used in technologies, medicine, aviation, civil engineering, etc. We describe the polyethylene creep under diffusion of liquid environment not interacting chemically with the polymer. The orthogonal functions can be used for approximation of characteristics obtained in analytical or experimental way. It is convenient because it is not necessary to re-calculate already determined coefficients in the expansion. This

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is the difference with regard to other algorithms where the change in the model order influences the values of all parameters. In this way the obtained coefficients in the expansion preserve their values for various representation domains - continuous and discrete, frequency and time as well as state space. The error of the model diminishes with increasing of its order. Since the series of the coefficients is distinguished by fast convergence, high precision of the model is obtained only by using the first few terms in the expansion (3) - (6) in the next paragraph.

The discussion on the assessment of the preciseness and influence of some parameters on a similar model while expanding impulse functions of the objects with delay (represented in orthogonal series) started in the work [7] (1974). Also we refer the reader to some useful notes on the general theory of functional differential equations with delay in [4], [6]. The approximation with Laguerre functions could be seen in [8] (1988). Some comments on the creep strength under viscoelastic conditions can be found in [1]-[2].

This work is written as follows:

Part 2 concerns some notes on the theory of the orthogonal expansions in modeling signal-dependent processes.

In Part 3 we present certain experimental data illustrating the process of viscoelastic deformation of polymer materials.

Part 4 is devoted to constructing a signal-dependent model for the integral components.

Determination of derivatives of the process under consideration as well as some important coefficients are given in Part 5 and 6.

Determination of correction vector is shown in Part 7.

The finding of analytical dependencies for some important quantities is shown in Part 8.

A number of important practical results can be found in Part 9.

2. Use of Orthogonal Expansions in Modeling Signal-Dependent Processes

It is assumed that the investigated evolution process is autonomous and its running in the interval $[0, t_f]$ depends on the vector $\lambda \in \mathbb{R}$, which is determined before the beginning of the process. The observed values for every running of the process represent the sum of useful signal $\eta(t)$ and noise $e(t)$:

$$y(\lambda, t) = \eta(\lambda, t) + e(t), \tag{1}$$

where $e(t)$ is white Gauss noise with zero mean and dispersion σ_ε^2. It is also assumed that the process $\eta(\lambda, t)$ is squared integrable in the interval $[0, t_f]$ for every value of λ, i.e. the function η belongs to the class $L([0, t_f])$ uniformly in $\lambda \in \mathbb{R}$, and in addition $\eta(\lambda, t) = 0$ whenever $t > t_f$. Then the function $\eta(\lambda, t)$ can be expanded in an infinite series of orthonormal functions $l_i(\alpha t)$

$$\eta(\lambda, t) = \sum_{i=1}^{\infty} \beta_i(\lambda) l_i(\alpha t), \tag{2}$$

where $\alpha > 0$ is a scaling factor, also $\alpha \in \mathbb{R}$, $l_i(\alpha t)$ - the i-th polynomial of Laguerre, that is, $l_i : \mathbb{R} \to \{\text{polynomials of Laguerrre}\}$. The property of orthonormality allows an independent determination of the values of the coefficients $\beta_i(\lambda)$ (see, e.g. [3], [8]) for each running of the process. It is known that

$$\beta_i(\lambda) = \int_0^{\infty} \eta(\lambda, t) l_i(\alpha t) dt, \qquad i = 1, 2, \ldots \tag{3}$$

If the function $\eta(\lambda, t)$ is continuous w.r.t. λ (that holds true for most of the applications, in which no change of the state is observed nonetheless the functional variables are changing), then the coefficients $\beta_i(\lambda)$ can be approximated with power series having the form

$$\beta_i(\lambda) = \sum_{j=0}^{m_i} b_{ij} \varphi_j(\lambda), \tag{4}$$

where the number of terms m_i depends on the extent of smoothness of $\beta_i(\lambda)$, and $\varphi(\lambda) \in \mathbb{R}$ are power functions of λ, that is, $\varphi_j : \{\lambda\} \subset \mathbb{R} \to \mathbb{R}$. Substituting (4) in (2) results in the generalized representation of the process $\eta(\lambda, t)$

$$\eta(\lambda, t) = \sum_{i=1}^{N} \sum_{j=0}^{m_i} b_{ij} \varphi_j(\lambda) l_i(\alpha t) \tag{5}$$

where the coefficients b_{ij} are unknown. By substituting in (5) the coefficients b_{ij} with their estimations and cutting the infinite functional series (2) the generalized model of the signal-dependent process is obtained:

$$\hat{y}(\lambda, t) = \sum_{i=1}^{N} \sum_{j=0}^{m_i} b_{ij} \varphi_j(\lambda) l_i(\alpha t), \tag{6}$$

where $\hat{y}(\lambda, t)$ is the predicted value of $\eta(\lambda, t)$. This equation describes quasi-stationary process for the respective values of λ. These values can be found experimentally (based on the reaction of step function) or analytically (based on the mechanism of the running processes). In this approach the model has separable properties – varying combination (depending on the signal impact) of stationary time functions.

Various systems of orthonormal functions are known in mathematics. In control theory the orthonormal polynomials of Laguerre have the most widespread application, and those of Walsh and others have limited use. In this case the Laguerre functions not only satisfy the requirements for approximation precision but also have simple Laplace images. Transformation in the frequency range and state space does not create problems. More general class of orthogonal functions are the Kautz functions (see [3]). They allow the use of complex poles and/or non-identical real poles in their structure but they require more computing power during the implementation.

An important assumption when applying Laguerre or Kautz functions is the squared integrable of the function. In this case the precision of approximation increases when the number of terms increases and this guarantees the convergence. Pertinent to the discussed topics is the case of Kautz for computing networks with non-identical real poles.

3. Description of the Process and the Experimental Data

Samples of polyethylene (PE for short) with high density are tested in liquid environment – cyclohexan which does not interact chemically with PE. Samples of PE at different levels of concentration of cyclohexan are tested under short creep in pure torsion and constant loading $-\sigma_{12} = 2.271$[MPa] (see, e.g. [1], [2]). The relative angular deformation ε_{12}[%] is taken into consideration. In order to simplify the model and the graphics the output quantity is represented as $\varepsilon = \varepsilon_{12} 10^4$.

On Figure 1 are presented graphically the output data for the deformation ε, at concentration C of cyclohexan at the following levels: 0%, 2.3%, 5.1% and 7.3%. Here and afterwards the curves are not denoted by numbers, the concentration is also not shown. It is enough to keep in mind that with the increase of concentration the deformation ε as well as the indicators derived from it increase (for one and the same value of time). An experiment is performed for one more concentration 3.5%, which was not considered during the processing of the results from the experiment for model building. It is used for a diagnos-

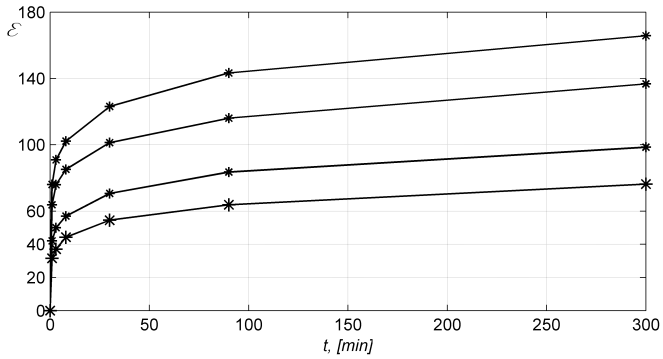

Figure 1: Experimental data for deformation (with $*$)

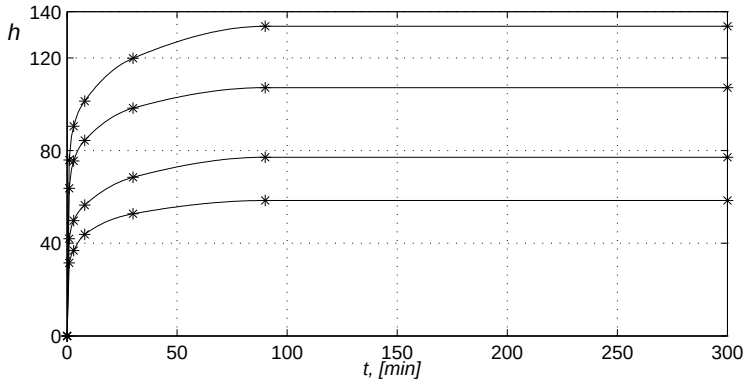

Figure 2: Deformation after removing the integral component

tic check of the obtained model and is compared to the model forecast (Figure 5). The following sections describe the steps of the algorithm through which the estimation of the orthogonal separable model goes. From the experimental data it is observed that after a definite period of time the speed of the process is constant. This means that:

1. The process contains the integral component which must be removed.

2. After removing the integral component, the reaction of step function does not satisfy the condition for squared integrable.

This is why a model of the derivative of the process will be sought as the functions will be replaced later with their integral functions.

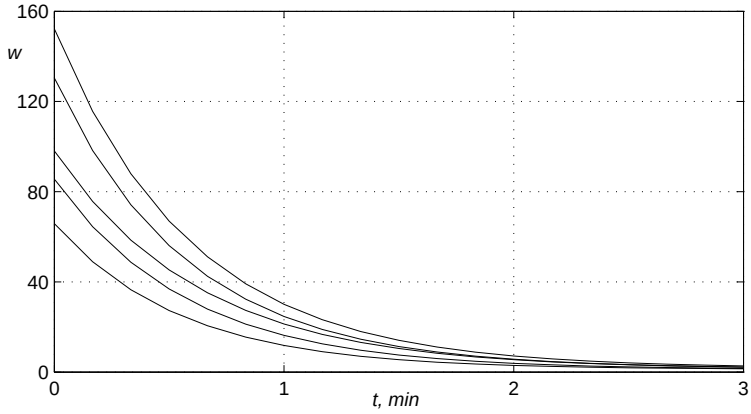

Figure 3: Derivatives of the process $w(C,t)$

4. Constructing a Signal-Dependent Model for the Integral Component

A model of this type is sought:

$$W_0(s,C) = \frac{k_u(C)}{s}, \tag{7}$$

where s is the argument of Laplace transform, $W_0(s,C)$ is a transfer function of the integration part of the system, $k_u(C)$ is the slope of an approximating line. When seeking analytic dependencies for $k_u(C)$ the choice is among the following three types of models:

— a linear model (with two coefficients),

— a polynomial model of second degree, in which three parameters are estimated

— an exponential model of the type:

$$k_u = \exp(a + b\ C), \tag{8}$$

where a and b are real constants.

In the third case the problem is reduced to a linear regression model with one factor and the dependent variable is $\ln k_n$.

If the coefficient of R^2- square statistic is significant, the model can be used for predictions. Otherwise, the model is inadequate. For comparison purposes in Table 1 are shown the residual sums of the squares of Q_R, common sum of

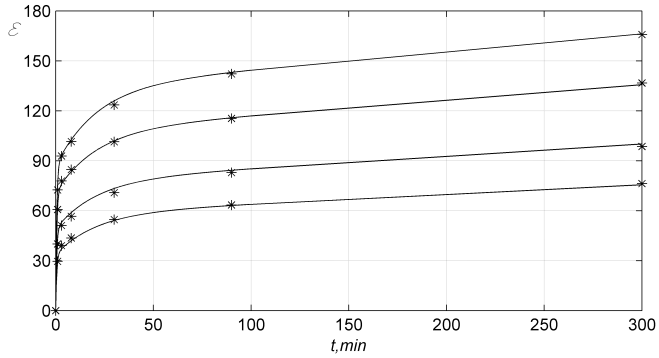

Figure 4: Output data (with) and predicted by the model-(with line)

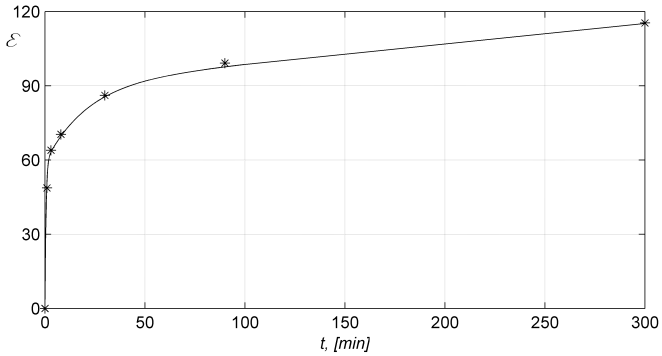

Figure 5: Comparison of the control experiment ($C = 3.5\%$) with and predicted by the model - with line

the squares of Q and the F-statistics for these models. Here F_T is the critical value of F - the Fisher criterion at level of significance $\alpha = 0.05$; $\nu_M = \kappa - 1$ and $\nu_R = n - k$ number of degrees of freedom; κ is the number of coefficients in the model. The number of experimental data is $n = 4$. In the considered case both the linear and the exponential model can be used for modeling the time constant of integration with approximately the same precision and have the form:

$$\hat{k_u}(C) = 0.0586 + 0.0069C \tag{9}$$

$$\hat{k_u}(C) = \exp\left(-2.8160 + 0.0850C\right) \tag{10}$$

After separating the integral component - the results are given in Figure 2

Comparison of models for the coefficient of integration $k_u(C)$ by statistical indicators					
Model type	k	Q	Q_R	Degrees of freedom	F-criterion $F_T(\alpha, \nu_1, \nu_2)$
1. Linear model	2	0,0015	1.77e-005	$\nu_M = 1$ $\nu_R = 2$	$F = 82.64$ $F_T = 18.51$
2. Second degree model	3	0.0015	3.40e-005	$\nu_M = 2$ $\nu_R = 1$	$F = 21.56$ $F_T = 199.5$
3. Exponential model	2	0.2267	0.003	$\nu_M = 1$ $\nu_R = 2$	$F = 73.17$ $F_T = 18.51$

Table 1

- for this part of the deformation is introduced the notation h_i, $i = 1, 2, 3, 4$.

$$h_i = h(C_i, t) = \varepsilon(C_i, t) - k_u(C_i)t \tag{11}$$

5. Determination of Derivatives of the Process

These four step responses - $h(C_i, t)$ are with self-settling but it is necessary to be differentiated when determining the arrays of coefficients (β_i). In the first 1 - 3 minutes when the speed of the processes is the highest, there is no additional information and a linear increase of the output quantity is assumed, i.e. the step responses most closely resemble these of first-order objects. The main difficulty comes from the small number of points and the high speed of deformation in the first few minutes, which are important for the precision of the modeling. Because of these reasons numerical differentiation is not applicable to the output data and neither are graphic and graph-analytic methods for approximation. For determining the derivatives $w(C, t)$ of the process the curves $h(C, t)$ (Figure 2) are approximated with sum of exponentials with non-linear optimization by the method of Nelder-Mead. As a result of this optimization the process is reduced to parallel connected two first-order objects, whose time constants are in the respective ranges: $T_1 = 21 \div 25$ [min], $T_2 = 0.58 \div 0.65$ [min]. Due to the high speed of the process in the initial period these derivatives are shown on Figure 3 only in the interval $0 - 3$ [min], after which they practically dump.

6. Determination of the Coefficients

The coefficients $\{\beta_i\}$ in (3) depend on the scaling factor α. The convergence of the series of coefficients $\{\beta_i\}$ depends weakly on the change of α in a given interval. This allows the achieving of very good approximation of impulse responses with different speed of dumping for a constant value of α [7]. From Figure 3 it seems that the choice of α in the range from 4 to 6 $[\text{min}]^{-1}$ provides a very good representation of the experimental data. The use of orthogonal model with Laguerre functions does not produce acceptable results because: the two time constants approximating the experimental data are very different which makes it possible the process to be very steep in the beginning but on the other hand to dump relatively slowly. That is why α cannot be chosen such that it can be used for approximation of the two first-order objects forming the model of deformation. As a result of all this, the use of Laguerre functions leads to correction coefficients $K_N(C_i)$ (by (12)) in the range 1.2 to 1.3 with number of terms in the expansion $N = 4$ to 6. That is why it is used a Kautz framework with non-identical real poles, $\alpha = [4.5 \;\; 4.5 \;\; 0.096 \;\; 0.096 \;\; 0.096 \;\; 0.096]$. In Table 2 are provided the first six Fourier coefficients. In this case the first three are enough, which is established experimentally - good convergence is achieved.

$\{\beta_i\}$	β_1	β_2	β_3	β_4	β_5	β_6
$C = 0\%$	32.3954	-6.7014	3.4983	0.3253	0.3631	0.3707
$C = 2.3\%$	45.9620	-7.1566	4.2620	0.0404	0.3029	0.3264
$C = 5.1\%$	68.8877	-11.7182	5.2313	0.4402	0.5598	0.5758
$C = 7.3\%$	82.7019	-13.7596	6.8020	0.2136	0.6515	0.6766

Table 2

7. Determination of the Correction Vector

The limited number N of participating in the approximation Kautz functions $\{K_i(\alpha_i, s)\}$ has to be considered when applying in practice the obtained here models. Since $N << \infty$ it can be expected that the requirements for coinciding of the beginning and the end of the true and the approximated function will not be kept. The static error is due to the finite number of terms in the series, due to the finite duration of realizations and mostly due to the noise which is superimposed in the initial data. Because of this when $t \to \infty$ a correction

coefficient $K_N(C)$ is introduced:

$$K_N(C) = \frac{h(C,\infty)}{\sum\limits_{i=1}^{N} \frac{2}{\sqrt{\alpha_i}}(-1)^{i-1}\beta_i(C)}, \tag{12}$$

where $h(C,\infty)$ is the already established value from (11).

When changing the number of the coefficients N, then K_N changes in order to avoid difference in the static behavior between the process and model. In Table 3 the correction coefficients $K_N(C_i)$ are calculated for $N = 1,\ldots,6$. After choosing N and calculating $\{\beta_i\}$ and K_N, the coefficients $\{\beta_i\}$ must be corrected:

$$\hat{\beta}_i(C) = K_N(C)\beta_i(C). \tag{13}$$

C_i / N	$N=1$	$N=2$	$N=3$	$N=4$	$N=5$	$N=6$
$C1=0\%$	1.9139	1.5859	0.9834	1.0194	0.9794	1.0203
$C2=2.3\%$	1.7803	1.5404	0.9943	0.9976	0.9730	0.9996
$C4=5.1\%$	1.6503	1.4104	0.9765	1.0024	0.9697	1.0034
$C5=7.3\%$	1.7143	1.4697	0.9912	1.0014	0.9709	1.0027

Table 3

In all following representations of the model input-output or in the state space we use the coefficients $\{\hat{\beta}_i\}$ instead $\{\beta_i\}$.

8. Finding Analytical Dependencies for $\hat{\beta}_i(C)$

Comparison of models for $\hat{\beta}_i(C)$ by statistical indicators						
Model type	R^2	F	F_T	ν_M	ν_R	s_R^2
Model 1	0.9980	986.16	18.51	1	2	1.51
Model 2	0.9445	0.34.04	18.51	1	2	1.51
Model 3	0.9911	223.27	18.51	1	2	0.00005

Table 4

For every one of the four step responses are calculated six coefficients $\hat{\beta}_i$, but only the first three are enough as shown by the values of the correction coefficients. The next step is determining the analytic expression for the coefficients

$$\hat{\beta}_i = \hat{\beta}_i(C, \theta), \qquad i = 1, 2, 3, \tag{14}$$

where C =const.

This problem is not trivial. For the considered process the following adequate models are determined:

1. Model for $\hat{\beta}_1(C)$: $\hat{\beta}_1(C) = 31.0794 + 6.9715\ C$
2. Model for $\hat{\beta}_2(C)$: $\hat{\beta}_1(C) = -5.8805 - 1.0384\ C$
3. Model for $\hat{\beta}_3(C)$: $\hat{\beta}_1(C) = [0.2869 - 0.0188\ C]^{-1}$

For comparison in Table 4 are provided the residual sums of the squares and the F- criterion of Fisher for these models. For all models the significance level is $\alpha = 0.05$, the number of experimental data is $N = 4$.

9. Results

1. In conclusion, an adequate model is obtained for a complex enough process. The model is separable and contains varying coefficients which depend on external independent signal/variable (in this case, the level of saturation of cyclohexan).

2. It is shown that when using orthogonal Laguerre and Kautz functions there is fast convergence of the series, from which it follows that only the first few terms of the expansion can be used. The decreased number of functions provides efficient way for storing the parameters of the model and for filtering of the object data while at the same time achieves satisfactory approximation. The structure of the model is convenient for practical application.

3. The possibility with orthogonal expansions to be approximated processes with/without self-settling substantially enlarges the areas of application of this approach because once established the dependencies of the coefficients are preserved in all areas of representation - time, frequency, discrete. Moreover, it is possible to use the framework of state space.

Acknowledgments

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References

[1] A. Alexandrov, Research mechanical proporties of structures, *Journal of the University of Chemical Technology and Metallurgy* (2003).

[2] A. Alexandrov, Tz. Tzolov, Creep strenght under viscoelastic conditions, *International Journal of Differential Equations and Applications*, **3** (2001), 359-363.

[3] D. Deschrijver, T. Dhaene, Data-driven model order reduction using orthonormal vector fitting, *Model Order Reduction: Theory, Research Aspects and Applications*, **13**, No. 3 (2008), 341-359.

[4] T. Donchev, N. Kitanov, D. Kolev, Stability for the solutions of parabolic equations with "maxima", *PanAmerican Mathematical Journal*, **20**, No. 2 (2010), 1-19.

[5] E. Jahnke, F. Emde, F. Lösch, *Tables of Higher Functions*, 6-th Ed. Revisited, McGraw-Hill, New York (1960).

[6] D. Kolev, N. Markova, Existence criteria for second order systems with "maxima", *International Electronic Journal of Pure and Applied Mathematics*, **1**, No. 3 (2010), 217-228.

[7] T. Petkov, P. Popov. Assessment of the preciseness and influence of the parameters of the model while expanding impulse functions of objects with delay in orthogonal series, In: *Assessment of Parameters and Models*, Central Council of Scientific-Technical Unions, Sofia (1974), 161-7, In Bulgarian.

[8] K. Velev, P. Popov, One opportunity for improving of approximation with Laguerre functions for realizations with finite duration, *Technical thought*, **3** (1988), In Bulgarian.