

IDENTIFICATION OF THE RELAXATION AND RETARDATION SPECTRA
OF PLANT VISCOELASTIC MATERIALS USING CHEBYSHEV FUNCTIONS
PART II. ANALYSIS

Anna Stankiewicz

Department of Technical Sciences
University of Life Sciences in Lublin

Summary. An optimal algorithm for the relaxation spectrum identification using discrete-time noise corrupted measurements of relaxation modulus obtained in stress relaxation test is proposed in the first part of the paper. The scheme is based on approximation of the spectrum of relaxation frequencies by the finite series of orthogonal Chebyshev functions optimal in the least-squares sense. Since the problem of relaxation spectrum identification is ill-posed inverse problem Tikhonov regularization with generalized cross validation (GCV) is used to guarantee the stability of the scheme. In this part of the paper an analysis of the model accuracy is conducted for noise measurements and the linear convergence of the approximations generated by the scheme is proved. It is also indicated that the accuracy of the spectrum approximation depends both on measurement noises and regularization parameter as well as on the proper selection of the time-scale parameter of the basic functions. A modification of the scheme for identification of retardation spectrum is also derived here. A numerical studies are the subject of the third part of the paper, where an example of the relaxation spectrum of a sample of the beet sugar root determination by applying the scheme proposed is also presented.

Keywords: Viscoelasticity, relaxation spectrum, retardation spectrum, identification, regularization, Chebyshev functions

INTRODUCTION

In the rheology it is commonly assumed that the relaxation modulus $G(t)$ has the following integral representation [Anderssen and Davies 2001, Christensen 1971]:

$$G(t) = \int_0^{\infty} H(\nu) e^{-\nu t} d\nu, \quad (1)$$

where: $H(\nu)$ is the spectrum of relaxation frequencies $\nu \geq 0$. Since, as it is well-known, for plant materials usually the long-term modulus $\lim_{t \rightarrow \infty} G(t) = G_{\infty} > 0$ (see [Jakubczyk i Lewicki 2003], as well as the Example 3 in the third part of the paper), instead of the classical equation (1), it is convenient to consider the following “more-realistic” augmented material description:

$$\bar{G}(t) = \int_0^{\infty} H(\nu) e^{-\nu t} d\nu + G_{\infty} \quad G(t) + G_{\infty} \quad (2)$$

In the first part of the paper an algorithm of the optimal least-squares approximation of the spectrum $H(\nu)$ by the finite series of (normalized) Chebyshev functions $\tilde{h}_k(\nu)$ (see (I.3)-(I.7), notation (I.3) is used for the eq. (3) in the first part of the paper):

$$H_k(\nu) = \sum_{k=0}^{K-1} g_k \tilde{h}_k(\nu), \quad (3)$$

where: g_k are constants, is proposed. The respective model $\bar{G}_k(t)$ (I.15) of the relaxation modulus $\bar{G}(t)$ is described by:

$$\bar{G}_k(t) = G_k(t) + G_\infty \sum_{k=0}^{K-1} g_k \phi_k(t) + G_\infty \quad (4)$$

where: the form of the functions $\phi_k(t)$ are given by Theorem 1 in the first part of the paper. A regularized scheme for computing the vector $g_k = [g_0 \dots g_{K-1} \ G_\infty]^T$ of optimal model parameters is presented in details in the first part of the paper. The scheme can be successfully applied to retardation spectrum identification; it is the subject of the subsequent section.

RETARDATION SPECTRUM IDENTIFICATION

An alternative to Boltzmann constitutive integral (I.1) linear viscoelastic constitutive equation expresses the strain $\varepsilon(t)$ in terms of the history of the time derivative of the stress $\dot{\sigma}(t)$ [Christensen 1971, Flügge 1967], i.e. the equation of convolution type:

$$\varepsilon(t) = \int_{-\infty}^t J(t-\tau) \dot{\sigma}(\tau) d\tau,$$

where: $J(t)$, $t \geq 0$, is the creep compliance (retardation function). For many viscoelastic materials, especially for soft biological materials as fruits and vegetables, the retardation function $J(t)$ is described by Kelvin (Kelvin-Voight) model of the form [Bzowska-Bakalarz 1994, Rao 1999]:

$$J(t) = J_0 + \int_0^\infty L(\nu) (1 - e^{-\nu t}) d\nu, \quad (5)$$

where: J_0 denote the time-independent (elastic) compliance and $L(\nu)$ is the spectrum of retardation frequencies, which characterises the distribution of retardation frequencies ν in the range $[\nu, \nu + d\nu]$ [Christensen 1971, Baumgaertel i Winter 1989, Stankiewicz 2005].

Retardation spectrum $L(\nu)$, like relaxation spectrum, is not directly accessible by experiment and thus must be determined from other material functions [Baumgaertel and Winter 1989, Elster et al. 1991, Bažant and Xi 1995, Emri and Tschoegl 1995, Ptaszek and Grzesik 2004]. The problem of spectrum $L(\nu)$ identification is the numerical problem of reconstructing solution of Fredholm integral equation of the first kind (5) with the kernel $(1 - e^{-\nu t})$ from discrete time-measured data [Engl 1993]. The practical difficulty in the identification of retardation spectrum, like for relaxation spectrum determination, is rooted in a theoretical mathematical problem difficulty, because it is ill-posed inverse problem [Groetsch 1993]. In this paper an optimal identification scheme of the least-squares approximation of the spectrum $L(\nu)$ by the linear combination of Chebyshev functions is proposed.

Assume that $L(\nu) \in L^2(0, \infty)$. The approximation of the retardation spectrum $L(\nu)$ by finite linear combination of the normalized basic Chebyshev functions $\tilde{h}_k(\nu)$ (I.7) is considered:

$$L_k(\nu) = \sum_{k=0}^{K-1} g_k (e^{2\alpha\nu} - 1)^{\nu/4} \tilde{h}_k(\nu) = \sum_{k=0}^{K-1} g_k \tilde{h}_k(\nu). \quad (6)$$

Then, the respective model of the retardation function $J(t)$, is described by:

$$J_k(t) = J_0 + \int_0^\infty L_k(\nu) (1 - e^{-\nu t}) d\nu = J_0 + \sum_{k=0}^{K-1} g_k \phi_k(t), \quad (7)$$

where the functions:

$$\phi_k(t) = \int_0^\infty h_k(\nu) (1 - e^{-\nu t}) d\nu, \quad (8)$$

and g_k are constants. The form of the basis functions $\phi_k(t)$ (8) for the retardation function model (7) is given by the following theorem; the proof is given in Appendix A.

Theorem 1. Let $\alpha > 0$ and $t \geq 0$. Then the basis functions $\phi_k(t)$ (8) are given by the recursive formula:

$$\phi_k(t) = 2\phi_{k-1}(t) + 4\phi_{k-1}(2\alpha) - 4\phi_{k-1}(t+2\alpha) - \phi_{k-2}(t), \quad k = 3, 4, \dots, \quad (9)$$

starting with:

$$\phi_0(t) = \frac{1}{\sqrt{2\alpha}} - \frac{1}{\sqrt{2\pi\alpha}} \frac{\Gamma(\frac{3}{4})\Gamma(\frac{t}{2\alpha} + \frac{1}{4})}{\Gamma(\frac{t}{2\alpha} + 1)}, \quad (10)$$

$$\phi_1(t) = \frac{1}{\sqrt{2\alpha}} - \frac{1}{2\alpha\sqrt{\pi\alpha}} \frac{\Gamma(\frac{3}{4})\Gamma(\frac{t}{2\alpha} + \frac{1}{4})}{\Gamma(\frac{t}{2\alpha} + 2)} [\alpha - t], \quad (11)$$

$$\phi_2(t) = \frac{1}{2\sqrt{2\alpha}} - \frac{1}{\sqrt{\pi\alpha}} \frac{\Gamma(\frac{3}{4})\Gamma(\frac{t}{2\alpha} + \frac{1}{4})}{4\alpha^2\Gamma(\frac{t}{2\alpha} + 3)} [t^2 + 2\alpha^2 - 6\alpha t] \quad (12)$$

A few first basis functions $\phi_k(t)$ (8) are shown in Figure 1 for two different values of the time-scaling factor α . It is evident that they are in good agreement with the retardation functions obtained in experiment.

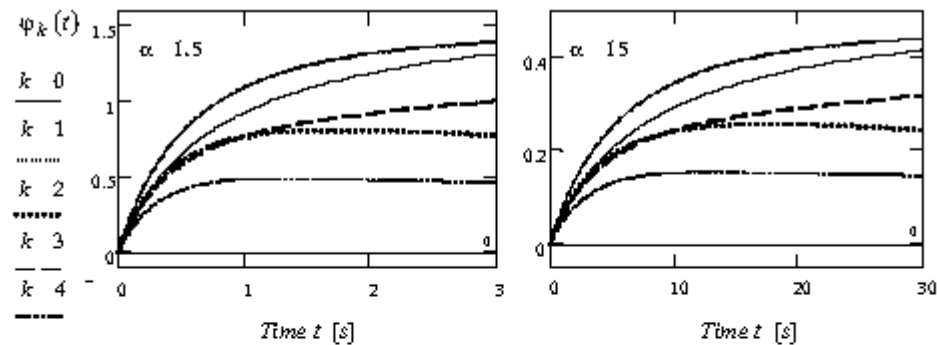


Fig. 1. Basic functions $\phi_k(t)$ of Chebyshev retardation spectrum identification algorithm, the parameters $\alpha = 1.5$ and $\alpha = 15$, $k = 0, 1, 2, 3, 4$

Suppose, a certain identification experiment (retardation test [Rao 1999]) performed resulted in a set of measurements of the retardation function $\bar{J}(t) = J(t) + z(t)$ at the sampling instants

$t_i \geq 0, i = 1, \dots, N$. As a measure of the model (7) accuracy the classical square index is taken [Bubnicki 1980], which introducing the convenient matrix-vector notation:

$$\Omega_{N,K} \begin{bmatrix} g_0(t_1) & \dots & g_{K-1}(t_1) & 1 \\ \vdots & \ddots & \vdots & \vdots \\ g_0(t_N) & \dots & g_{K-1}(t_N) & 1 \end{bmatrix} \quad \bar{J}_N \begin{bmatrix} \bar{J}(t_1) \\ \vdots \\ \bar{J}(t_N) \end{bmatrix}$$

we could write as:

$$Q_N(g_K) = \sum_{i=1}^N [\bar{J}(t_i) - J_K(t_i)]^2 = \|\bar{J}_N - \Omega_{N,K} g_K\|_2^2$$

where: $g_K = [g_0 \dots g_{K-1} J_0]^T$ is $(K+1)$ -element vector of the models (6) and (7) parameters. Thus the optimal identification of retardation spectrum in the class of functions $L_K(\nu)$ given by (6) consists of solving, with respect to the model parameter g_K , the classical least-squares problem [Lawson i Hanson 1995]. This problem, analogously to the previous optimal identification of the relaxation spectrum task, could be solved by applying the scheme proposed in the first part of the paper, replacing the matrix $\Phi_{N,K}$ by $\Omega_{N,K}$ and substituting the creep compliance measurements vector J_N instead of G_N .

ANALYSIS

Smoothness

By orthonormality of the basic Chebyshev functions $\{\tilde{h}_k(\nu)\}$ in the space $L^2(0, \infty)$ [Szabat 1982], for an arbitrary $H_K(\nu)$ of the form (3) the following equality holds:

$$\|H_K\|_2^2 = \sum_{k=0}^{K-1} \sum_{j=0}^{K-1} g_k g_j \int_0^\infty \tilde{h}_k(\nu) \tilde{h}_j(\nu) d\nu = \sum_{k=0}^{K-1} g_k^2 = \|g_K\|_2^2 \quad (13)$$

here: $\|\cdot\|_2$ means also the square norm in $L^2(0, \infty)$. Therefore, due to the basic Chebyshev functions orthonormality the smoothness of the regularized solution g_K^L (I.20) guarantees that the fluctuations of the respective relaxation spectrum $\hat{H}_K(\nu)$ (I.27) are bounded.

Stabilization

The purpose of the regularization [Tikhonov and Arsenin 1977] relies on stabilization of the resulting vector g_K^L (I.20). The effectiveness of this approach can be evaluated by the following relations, which follow immediately from Proposition 2.2 in [Stankiewicz 2007].

Proposition 1. Let $K \geq 1$, $r = \text{rank}(\Psi_{K,K})$ and regularization parameter $\lambda > 0$. For the regularized solution g_K^L (I.20) the following equality and inequality hold:

$$\|g_K^L\|_2^2 = \sum_{i=1}^r \frac{y_i^2}{(\sigma_i + \lambda)^2} < \sum_{i=1}^r \frac{y_i^2}{\sigma_i^2} = \|\bar{g}_K^N\|_2^2, \quad (14)$$

where: $\bar{g}_K^N$ is the normal solution of the linear-quadratic problem (I.17)-(I.18), y_i are the elements of the vector $Y = V^T \Phi_{N,K}^T \bar{G}_N$ and σ_i are non-zero singular values of the matrix $\Psi_{K,K} = \Phi_{N,K}^T \Phi_{N,K}$ (for details see the first part of the paper).

The first equality in (14) illustrates the mechanism of stabilization. The following rule holds: the greater the regularization parameter λ is, the fluctuations of the vector g_x^{λ} are highly bounded. Thus, the regularization parameter controls the “smoothness” of the regularized solution.

Measurement noises

The influence of the measurement noises on the regularized vector g_x^{λ} (1.24) is discussed in details in the Appendix C.4 in the thesis [Stankiewicz 2007]. Suppose:

$$\tilde{g}_x^{\lambda} = V \Omega_1 V^T \Phi_{N,K}^T G_N \quad (15)$$

where: $G_N = [G(t_1) \dots G(t_N)]^T$ is the noise-free measurement data, be the regularized vector for data G_N . On the basis of Property C.4 in [Stankiewicz 2007] the next proposition is stated.

Proposition 2. Let $K \geq 1$, $r = \text{rank}(\Psi_{x,K})$ and $\lambda > 0$. For g_x^{λ} the following estimations hold:

$$\|g_x^{\lambda} - \tilde{g}_x^{\lambda}\|_2 \leq \max_{1 \leq i \leq r} \frac{\sqrt{\sigma_i}}{(\sigma_i + \lambda)} \|z_N\|_2 \leq \frac{\sqrt{\sigma_1}}{(\sigma_r + \lambda)} \|z_N\|_2,$$

where: $z_N = [z(t_1) \dots z(t_N)]^T$ is the disturbances vector, thus the regularized vector g_x^{λ} tends to regularized solution for noise-free measurements linearly with respect to the noises z_{t_i} as $\|z_{t_i}\|_2 \rightarrow 0$.

Convergence

Let us estimate the regularized vector $g_x^{\lambda_{CCV}}$ error, i.e. the norm $\|g_x^{\lambda_{CCV}} - g_x^N\|_2$, where g_x^N is the normal solution of the least-squares task (I.17)-(I.18) for noise-free data G_N . Relaxation spectrum $\hat{H}_K(\nu) = \sum_{k=0}^{K-1} g_k^{\lambda_{CCV}} \tilde{h}_k(\nu)$ (I.27) is only approximation of that spectrum, which can be obtained in the chosen class of models (I.8) by direct minimization (without regularization) of the quadratic quality index (I.17) for noise-free measurements, i.e. the approximation of the function $H_K^N(\nu) = \sum_{k=0}^{K-1} g_k^N \tilde{h}_k(\nu)$, where g_k^N are the elements of the vector g_x^N . The accuracy of the spectrum approximation depends both on the measurement noises and the regularization parameter λ as well as on the singular values of the matrix $\Psi_{x,K}$ which, in turn, depend on the proper selection of the time-scale factor a of the Chebyshev functions $\tilde{h}_k(\nu)$. The above is evident by the next proposition which can be easily derived from Property 2.5 in [Stankiewicz 2007] using the equality in (13).

Proposition 3. Let $K \geq 1$, $r = \text{rank}(\Psi_{x,K})$ and $\lambda > 0$. The following equality and inequality hold:

$$\|\hat{H}_K - H_K^N\|_2 = \|g_x^{\lambda_{CCV}} - g_x^N\|_2 \leq \sum_{i=1}^r \frac{\lambda_{CCV} |y_i|}{\sigma_i (\sigma_i + \lambda_{CCV})} + \frac{1}{\sigma_r} \|z_N\|_2 \quad (16)$$

therefore, the regularized vector $g_x^{\lambda_{CCV}}$ converges to the normal solution g_x^N and the relaxation spectrum $\hat{H}_K(\nu)$ tends to the “normal” spectrum $H_K^N(\nu)$ in each point ν at which they are both continuous, linearly with respect to the norm $\|z_N\|_2$ as $\lambda_{CCV} \rightarrow 0$ and $\|z_N\|_2 \rightarrow 0$, simultaneously.

FINAL REMARK

The inequality (16) yields that the accuracy of the spectrum approximation depend both on the measurement noises and the regularization parameter as well as on the singular values $\sigma_1, \dots, \sigma_r$ of the matrix $\Phi_{N,K}$ (I.18), which, in turn, depend on the proper selection of the basic Chebyshev functions.

APPENDIX A

Proof of Theorem 1. Suppose $\alpha > 0$. It is easy to observe that the integral $\phi_k(t)$ (8) can be expressed as a difference of two integrals:

$$\phi_k(t) = \int_0^\infty \tilde{h}_k(\nu) d\nu - \int_0^\infty \tilde{h}_k(\nu) e^{-\alpha\nu} d\nu = \phi_k(0) - \phi_k(t), \quad (\text{A.1})$$

where: the function $\phi_k(t)$ is defined by the eq. (I.10). Whence, for $k=0$ we have:

$$\phi_0(t) = \phi_0(0) - \phi_0(t) = \frac{1}{\sqrt{2\pi\alpha}} \frac{\Gamma(\frac{3}{4})\Gamma(\frac{1}{4})}{\Gamma(1)} - \frac{1}{\sqrt{2\pi\alpha}} \frac{\Gamma(\frac{3}{4})\Gamma(\frac{1}{4} + \frac{1}{2\alpha})}{\Gamma(\frac{1}{2\alpha} + 1)}.$$

Since $\Gamma(1) = 1$, and on the basis of known Euler's gamma function identity $\Gamma(z)\Gamma(z + \frac{1}{2}) = 2^{1-2z}\Gamma(2z)$ [Lebiedew 1957] we have:

$$\Gamma(\frac{3}{4})\Gamma(\frac{1}{4}) = 2^{1/2}\Gamma(\frac{1}{2}) = \sqrt{2\pi}, \quad (\text{A.2})$$

because $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, we finally receive eq. (10). Likewise for $k=1$, combining the equations (A.1), (I.13), (A.2) and the fact that $\Gamma(2) = 1$ we obtain eq. (11). To prove (12) for $k=2$ it is enough to substitute (I.14) into (A.1) taking into account (A.2) and $\Gamma(3) = 1$.

We next show that (9) holds for any $k \geq 3$. Using the identity (I.A.2) and the defining formula (8) we now have:

$$\phi_k(t) = 2 \int_0^\infty \tilde{h}_{k-1}(\nu) (1 - e^{-\alpha\nu}) d\nu - 4 \int_0^\infty e^{-2\alpha\nu} \tilde{h}_{k-1}(\nu) (1 - e^{-\alpha\nu}) d\nu - \int_0^\infty \tilde{h}_{k-2}(\nu) (1 - e^{-\alpha\nu}) d\nu,$$

and hence, taking into account again the definition (8), we obtain:

$$\phi_k(t) = 2\phi_{k-1}(t) - 4 \int_0^\infty \tilde{h}_{k-1}(\nu) e^{-2\alpha\nu} d\nu + 4 \int_0^\infty \tilde{h}_{k-1}(\nu) e^{-2\alpha\nu} e^{-\alpha\nu} d\nu - \phi_{k-2}(t).$$

Hence by virtue of the basic functions $\phi_k(t)$ definition (I.10) we have:

$$\phi_k(t) = 2\phi_{k-1}(t) - 4\phi_{k-1}(2\alpha) + 4\phi_{k-1}(t+2\alpha) - \phi_{k-2}(t),$$

and since noting that by virtue of (A.1) $\phi_k(t) = \phi_k(0) - \phi_k(t)$ we conclude that the eq. (9) is valid. The proof is now complete.

REFERENCES

- Anderssen R. S., Davies A. R. 2001.: Simple moving-average formulae for the direct recovery of the relaxation spectrum. *Journal of Rheology* 45, 1-27.
- Baumgaertel M., Winter H. H. 1989.: Determination of discrete relaxation and retardation time spectra from dynamic mechanical data. *Rheological Acta* 28, 511-519.
- Bažant Z.P., Xi Y. 1995.: Continuous retardation spectrum for solidification theory of concrete creep. *J. of Engrg. Mech. ASCE* 121 (2), 281-288.
- Bubnicki Z. 1980.: Identification of Control Plants. PWN Warszawa, Elsevier Amsterdam.
- Bzowska-Bakalarz M. 1994.: Właściwości mechaniczne korzeni buraków cukrowych. Rozprawy Naukowe Akademii Rolniczej w Lublinie, 166.
- Christensen R.M. 1971.: Theory of Viscoelasticity. An Introduction. Academic Press, New York.

- Elster C., Honerkamp J., Weese J. 1991.: Using regularization methods for the determination of relaxation and retardation spectra of polymeric liquids. *Rheological Acta*, 30, 161-174.
- Engl H. W. 1993.: Regularization methods for the stable solution of inverse problems. in: *Surveys Math. for Industry*, Springer, Austria.
- Emri I., Tschögl N. W. 1995.: Determination of mechanical spectra from experimental response. *International Journal of Solids and Structures*, 32(6/7), 817-826.
- Flügge W. 1967.: *Viscoelasticity*. Blaisdell Publishing Company Waltham, Toronto, London.
- Groetsch C. W. 1993.: *Inverse Problems in the Mathematical Sciences*, Vieweg Publishing, Wiesbaden.
- Jakubczyk E., Lewicki P. P. 2003.: Własności mechaniczne tkanki jabłka w odniesieniu do jej struktury. *Acta Agrophysica* 2(3), 549-557.
- Lawson C. L., Hanson R. J. 1995.: *Solving Least Squares Problems*. Prentice-Hall, Englewood Cliffs, NJ, 1974; reprinted by SIAM, Philadelphia, PA.
- Lebiedew N.N. 1957.: *Funkcje specjalne i ich zastosowania*. PWN, Warszawa.
- Ptaszek P., Grzesik M. 2004.: Lepkosprężyste zjawiska retardacyjne w modelowym układzie skrobia kukurydziana-guma guar. *Acta Agrophysica*, 3(3), 573-578.
- Rao M.A. 1999.: *Rheology of Fluid and Semisolid Foods. Principles and Applications*. Aspen Publishers, Inc., Gaithersburg, Maryland.
- Stankiewicz A., 2005.: Approximation of the retardation spectrum of plant viscoelastic materials using Legendre functions. *Acta Agrophysica* 6(3), 795-813 (in Polish).
- Stankiewicz A. 2007.: Identyfikacja spektrum relaksacji lepkosprężystych materiałów roślinnych. Rozprawa doktorska, Akademia Rolnicza w Lublinie, Lublin.
- Szabatn J. 1982.: *Podstawy teorii sygnałów*. Wyd. Komunikacji i Łączności, Warszawa.
- Tikhonov A.N., Arsenin V.Y. 1977.: *Solutions of Ill-posed Problems*. John Wiley and Sons New York, USA.

IDENTYFIKACJA SPEKTR RELAKSACJI I RETARDACJI LEPKOSPŘŻYSTYCH MATERIAŁÓW ROŚLINNYCH Z WYKORZYSTANIEM FUNKCJI CZEBSZEW CZĘŚĆ II. ANALIZA

Streszczenie. W pierwszej części pracy zaproponowano algorytm optymalnej identyfikacji spektrum relaksacji na podstawie dyskretnych pomiarów modułu relaksacji zgromadzonych w dziedzinie czasu w teście relaksacji naprężeń. Schemat bazuje na aproksymacji spektrum częstotliwości relaksacji skończoną sumą ortogonalnych funkcji Czebyszewa optymalnej w sensie najmniejszej sumy kwadratów. Ponieważ problem identyfikacji spektrum relaksacji jest źle postawionym problemem odwrotnym dla zapewnienia stabilności rozwiązania zastosowano regularyzację Tichonowa i uogólnioną metodę sprawdzania krzyżowego (GCV). W tej części pracy przeanalizowano dokładność modelu dla załdconych pomiarów modułu relaksacji oraz wskazano na liniową zbliżność modelu do modelu jaki uzyskalibyśmy dla pomiarów idealnych. Pokazano także, że dokładność przybliżenia spektrum relaksacji zależy zarówno od błędów pomiarowych oraz parametru regularyzacji jak również od odpowiedniego doboru współczynnika skali czasu funkcji bazowych. W pracy zaproponowano także modyfikację schematu dla zadania identyfikacji spektrum retardacji. Badania numeryczne są przedmiotem trzeciej części pracy, w której przedstawiono także obok przykładu symulacyjnego przykład jej zastosowania do wyznaczenia spektrum relaksacji rzeczywistego materiału pochodzenia roślinnego.

Słowa kluczowe: lepkosprężystość, spektrum relaksacji, spektrum retardacji, identyfikacja, regularyzacja, funkcje Czebyszewa