

IDENTIFICATION OF THE RELAXATION AND RETARDATION
SPECTRA OF PLANT VISCOELASTIC MATERIALS
USING CHEBYSHEV FUNCTIONS
PART III. NUMERICAL STUDIES AND APPLICATION EXAMPLE

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Summary. The optimal scheme of the least-squares approximation of the spectrum of relaxation frequencies by the finite series of orthogonal Chebyshev functions is proposed in the first part of the paper. The spectrum is recovered from discrete-time noise corrupted measurements of relaxation modulus obtained in stress relaxation test. Theoretical analysis of the model accuracy, convergence of the scheme and the influence of the measurement noises on the model determined is the subject of the second part of the paper. In this paper the validity and effectiveness of the method is demonstrated using simulated data of Gaussian relaxation spectrum. Numerical calculations on model data are presented. Applying the scheme proposed, the relaxation spectrum of an unconfined cylindrical specimen of the beet sugar root is determined.

Keywords: Relaxation spectrum, identification, regularization, Chebyshev functions

INTRODUCTION

The selection of an appropriate mathematical representation is of central importance in the analysis of a physical system. Often the choice of the respective model depend on essentially two criteria: the particular characteristics to be abstracted and, perhaps more importantly, our ability to specify the representation quantitatively. System identification deals with the problem of building mathematical models of dynamical systems (processes) based on observed data from the system. In order to find such a model, which good (in the best) describe the system (process) an appropriate identification method must be derived [Mańczak and Nahorski 1983, Ljung 1999].

A complication for determining the relaxation and retardation spectra, is that these problems are undetermined and ill-conditioned in the Hadamard sense [Honerkamp 1989, Orbey and Dealy 1991]. Due to the noise or truncation of the experimental data, many models may fit the relaxation modulus or creep compliance experimental data adequately, but small errors in the data may lead to large changes in the models determined. Thus the practical difficulty in the identification of these models is rooted in a theoretical difficulty. The mathematical difficulties can be overcome by synthesis of an appropriate identification algorithm.

In the first part of the paper new optimal scheme of the least-squares approximation of the spectrum $H(\nu)$ of relaxation frequencies $\nu \geq 0$ by the linear combination of (normalized) Chebyshev functions $\tilde{h}_k(\nu)$ (see (1.3)-(1.7), notation (1.3) is used for the eq. (3) in the first part of the paper):

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

where: g_k are constants, on the basis of noise corrupted time-measurements of relaxation modulus $G(t)$ is proposed. Tikhonov regularization is used to guarantee the stability of the scheme for computing the vector $g_k = [g_0 \dots g_{K-1} \ G_\infty]^T$ of optimal model parameters [Tikhonov and Arsenin 1977]. Generalized cross validation (GCV) is adopted for the optimal choice of the regularization parameter [Heinz and Martin 1996]. The numerical realization of the schemes by using the singular value decomposition (SVD) is discussed [Björck 1996] and the resulting computer algorithm is also outlined in the first 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 in the second part of the paper. 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 parameters of basic functions.

In this part of the paper the results of the numerical studies are presented. In the context of the ill-posed inverse problem for which the model quality index refer to the measured relaxation modulus but not directly to the unknown relaxation spectrum such simulation allow beside theoretical analysis demonstrate the validity and effectiveness of the method [Varah 1983, Tautenhahn 1994]. The experiment simulations are conducted using Gaussian relaxation spectrum. Such an example illustrates most of the works concerning relaxation or retardation spectrum identification, for example [Elster et al. 1991, Syed Mustapha and Phillips 2000]. Both asymptotic properties of the scheme as well as the influence of the measurement noises on regularized solution are examined.

NUMERICAL STUDIES

Example 1. Consider viscoelastic material whose relaxation spectrum is described by the Gauss distribution:

$$H(\nu) = \frac{1}{6\sqrt{2\pi}} e^{-(\nu/20)^2/72}. \quad (2)$$

The corresponding relaxation modulus is described by:

$$G(t) = \frac{1}{2} e^{-20\alpha + 18t^2} \operatorname{erfc}(3\sqrt{2}t - 5\sqrt{2}/3), \quad (3)$$

where: $\operatorname{erfc}(t)$ is complementary error function [Lebiediew 1957]. The relaxation spectrum $H(\nu)$ (2) is given in figure 2(b) (dashed line). In experiment the sampling instants t was generated with the constant period in time interval $T = [0, 0.4]$ selected in view of the relaxation modulus $G(t)$ (3) course. Additive measurement noises $\{z_i\}$ was selected independently by random choice with uniform distribution on the interval $[-0.003, 0.003]$, i.e. 5% of the mean value of the modulus $G(t)$ maximally. For every pair (K, N) of the range $K=4, 6, 7, 8$ and $N=50, 100, 500, 1000, 5000, 10000$ the experiment was repeated $n=100$ times.

Approximation error of the relaxation modulus measurements

To estimate the approximation error of the relaxation modulus measurements for n -element sample the following index (cf. the index $Q_N(g_k)$ (I.17)) is taken:

$$ERR_{Q_N-LS}(N, K) = \frac{1}{nN} \sum_{j=1}^n Q_N(g_{k,j}^A) = \frac{1}{nN} \sum_{j=1}^n \left\| \bar{G}_N - \Phi_{N,j} g_{k,j}^A \right\|_2^2, \quad (4)$$

where: $\Phi_{N,j}$ denote the matrix $\Phi_{N,k}$ (I.18) and $g_{k,j}^A$ (I.20) is the regularized model parameter determined for j -th experiment repetition for a given pair (N, K) , $j = 1, \dots, n$. Here $\left\| \cdot \right\|_2$ means the square norm in the Euclidean space R^N . The index $ERR_{Q_N-LS}(N, K)$ as a function of the model summands K and the number of measurements N is depicted in figure 1(a). Time-scale factor $\alpha = 0.05$ and the regularization parameter $\lambda_{GCP} \approx 0.0001$ were taken; they were valid in all the simulation experiment. For $K \geq 6$ the algorithm ensures very good quality of the modulus measurements approximation even for $N \geq 50$ because the error index $ERR_{Q_N-LS}(N, K)$ is comparable with the normal solution error for noise-free measurements. The index $ERR_{Q_N-LS}(N, K)$ does not depend essentially on the number of measurements.

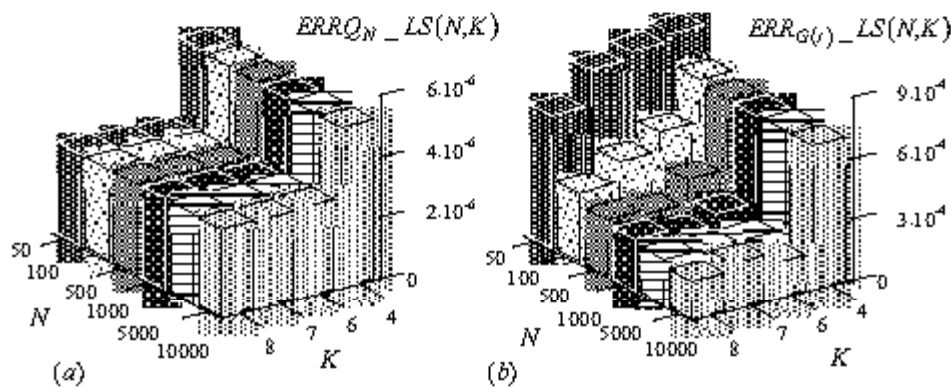


Fig. 1. (a) The mean square approximation error of the modulus measurements $ERR_{Q_N-LS}(N, K)$ (4);
(b) Integral approximation error of the relaxation modulus $ERR_{G(t)-LS}(N, K)$ (5)

Integral approximation error of the relaxation modulus

As a measure of the approximation of the true relaxation modulus $G(t)$ (3) the mean integral approximation error defined as:

$$ERR_{G(t)-LS}(N, K) = \frac{1}{n} \sum_{j=1}^n Q(g_{k,j}^A) \quad (5)$$

where: $Q(g_k^A) = \int_0^\infty [G(t) - G_k(t)]^2 dt$ is taken. The index $ERR_{G(t)-LS}(N, K)$ (5) as a function of K and N is given in figure 1(b). Very good approximation of the true relaxation modulus is achieved even for $K \geq 6$; the better the greater is the number of model summands and the number of

measurement points. Since $\int_0^\infty G(t)^2 dt = 0.0262768475$, the relative true modulus approximation error for $K \geq 6$ and $N \geq 500$ is included in the range from 0.688% to 0.832%.

Integral approximation error of the relaxation spectrum

The mean integral error of the true relaxation spectrum $H(\nu)$ approximation defined as:

$$ERR_{H(\nu)} - LS(N, K) = \frac{1}{n} \sum_{j=1}^n Q\nu(g_{K,j}^A), \quad (6)$$

where: $Q\nu(g_K^A) = \int_0^\infty [H(\nu) - H_K(\nu)]^2 d\nu$ is the global integral error of the true spectrum approximation, has been determined. For $K \geq 6$ the error $ERR_{H(\nu)} - LS(N, K)$ is decreasing function of the number of sampling points and the number of model summands as depicted in figure 2(a).

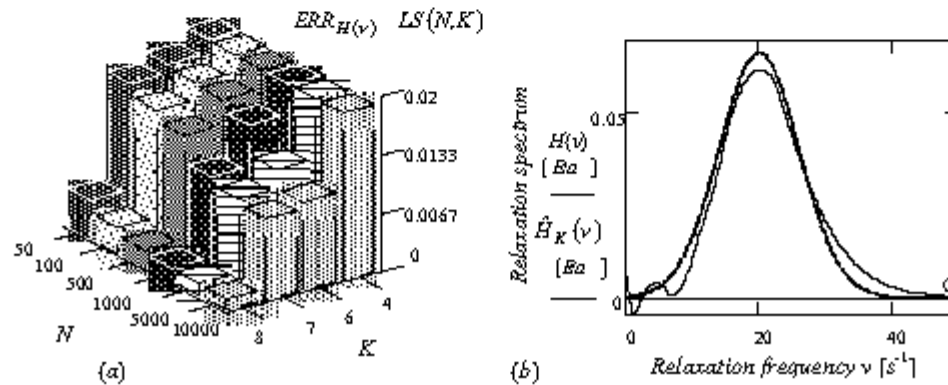


Fig. 2 (a) Integral error of the relaxation spectrum approximation $ERR_{H(\nu)} - LS(N, K)$ (6); (b) Relaxation spectrum $H(\nu)$ (2) (dash line) and the approximated model $\hat{H}_K(\nu)$ (solid line).

The best approximation error is achieved for $K=8$. Since $\int_0^\infty H(\nu)^2 d\nu = 0.0470157$, the relative approximation error of the true relaxation spectrum for $K=8$ and $N \geq 1000$ is included in the range 0.034–0.0255, i.e. that is not exceed 4%. The approximation quality can be improved by proper choice of the regularization parameter as well as the time-scale factor a (see Remark 4 in the first part of the paper).

Measurement noise influence

In order to study the influence of the noise variance σ^2 on the vector of model parameters the experiment have been repeated $n=500$ times. Noises have been generated independently by random choice with uniform distribution on the interval $[-h, h]$ for $h = 0.0005, 0.001, 0.005, 0.01$, $N = 50, 100, 500, 1000, 5000, 10000$ and $K = 6, K = 8$. $h = 0.01$ is 1% of the maximum value of $G(t)$ and $h = 0.0005$ is about 1% of the mean value of the modulus. Such measurement noises are even strongest than the “true” disturbances recorded for the plant materials (see [Stankiewicz 2007, Chapter 5.5.4]). For example for the sugar beet sample from example 3 disturbances have not ex-

ceeded 0.8% of the maximum value of $G(t)$ and have not exceeded 0.7% of the mean value of the modulus. The distance between \mathbf{g}_K^A and the regularized solution for noise-free measurements $\tilde{\mathbf{g}}_K^A$ (II.15) has been estimated by normalized mean error defined for n element sample as:

$$ERR(N, K, \sigma^2) = \frac{1}{n} \sum_{j=1}^n \|\mathbf{g}_{Kj}^A - \tilde{\mathbf{g}}_{Kj}^A\|_2 / \|\tilde{\mathbf{g}}_{Kj}^A\|_2. \quad (7)$$

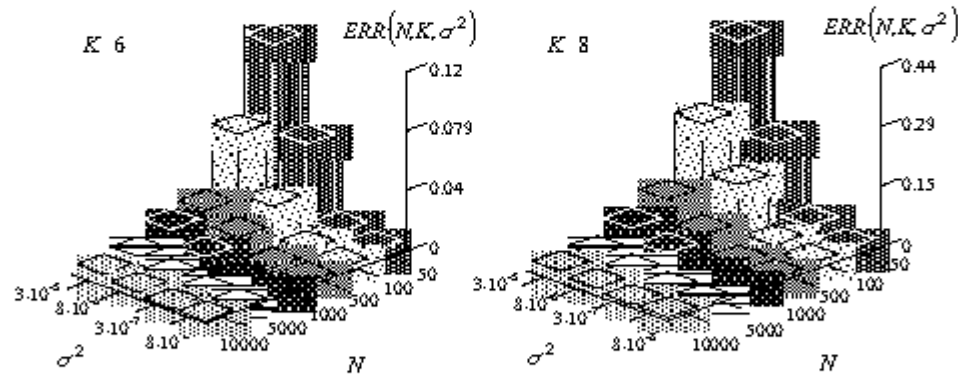


Fig. 3. The index $ERR(N, K, \sigma^2)$ as a function of N and σ^2 for $K=6$ and $K=8$

Since in the experiment the sampling period has been constant the vector $\tilde{\mathbf{g}}_{Kj}^A$ does not depend on j , i.e. $\tilde{\mathbf{g}}_{Kj}^A = \tilde{\mathbf{g}}_K^A$. Relationship of $ERR(N, K, \sigma^2)$ (7) on N and σ^2 is depicted in figure 3. The index $ERR(N, K, \sigma^2)$ depends on the noise variance as well as on the matrix $\Phi_{N,K}$ (i.e. on the numbers of model summands and the measurements) and on the regularization parameter. For satisfactory large number of measurements ($N \geq 1000$) the index $ERR(N, K, \sigma^2)$ do not exceed 7% even for large noises and $K=8$.

The ranges of variation of the approximation error indices used in the simulation experiment are given in table 1. The next two examples show how the scheme proposed can be used in the relaxation spectrum identification.

NUMERICAL EXAMPLE

Example 2. Let us suppose again that the true relaxation spectrum is described by the Gauss distribution $H(\nu)$ (2). The relaxation modulus $\bar{G}(t) = G(t) + z(t)$ corrupted by additive measurement noises $z(t)$ of the uniform distribution in the interval $[-0.02, 0.02]$ has been sampled at $N=500$ sampling instants at the constant period $\Delta t = 0.0012s$. The parameters $K=8$ and $\alpha = 0.25s$ are chosen according to the suggestions of Remark 4 in the first part of the paper. The “true” relaxation spectrum $H(\nu)$ (2) and the resulting approximated model $\hat{H}_K(\nu)$ (1.27) are plotted in figure 2(b).

Table 1. The ranges of variation of the approximation error indices used in the simulation experiment

	$K=4$	$K=6$	$K=7$	$K=8$
$ERR_{\sigma} LS(N,K)$	8.679E-6÷8.81E-6	2.67E-6÷3.039E-6	2.633E-6,3.01E-6	2.62E-6÷3.002E-6
$ERR_{\sigma_0} LS(N,K)$	7.077E-4÷8.95E-4	1.807E-4÷8.55E-4	2.185E-4÷8.16E-4	1.88E-4÷6.458E-4
$ERR_{\eta_0} LS(N,K)$	0.0189÷0.0193	9.978E-3÷0.018	9.167E-3÷0.017	1.2E-3÷4.518E-3
$ERR(N,K,\sigma^h)$	$h = 0.0005$	$h = 0.001$	$h = 0.005$	$h = 0.01$
$K=6$	3.2778E-4÷0.0063	6.5985E-4÷0.0106	0.0033÷0.0607	0.0072÷0.1186
$K=8$	0.0012÷0.0195	0.0025÷0.0432	0.0116÷0.2153	0.0241÷0.4386

RELAXATION SPECTRUM OF THE SUGAR BEET SAMPLE

Example 3. A cylindrical sample of 20 mm diameter and height was obtained from the root of sugar beet Janus variety [Gołacki et al. 2003]. During the two-phase stress relaxation test, in the first initial phase the strain was imposed instantaneously, the sample was preconditioned at the $0.5 \text{ m} \cdot \text{s}^{-1}$ strain rate to the maximum strain. Next, during the second phase at constant strain the corresponding time-varying force induced in the specimen was recorded during the time period $[0,100]$ seconds in 40000 measurement points with the constant period $\Delta t = 0.0025 \text{ s}$. Only $N = 958$ points were taken

for identification purposes with the time period $\Delta t_i = 0.1$ s for $0.5 \leq t \leq 96.2$ s. The experiment was performed in the state of uniaxial stress; i.e. the specimen examined underwent deformation between two parallel plates. Modelling mechanical properties of this material in linear-viscoelastic regime is justified by the research results presented in a lot of works, for example [Bzowska-Bakalarz 1994, Gołacki 2002]. The respective relaxation modulus was computed using the modification of the well-known Zapas and Craft rule [Zapas and Phillips 1971, Flory i McKenna 2004] derived in [Stankiewicz 2007]. Next the proposed identification scheme was applied and the relaxation spectra obtained are plotted in figure 4 for two samples. For both samples $K = 8$ and $\alpha = 75$ s was chosen, the long-term modulus was as follows $G_\infty = 8.1914$ MPa and $G_\infty = 9.0529$ MPa (see Augmented Model section in the first part of the paper).

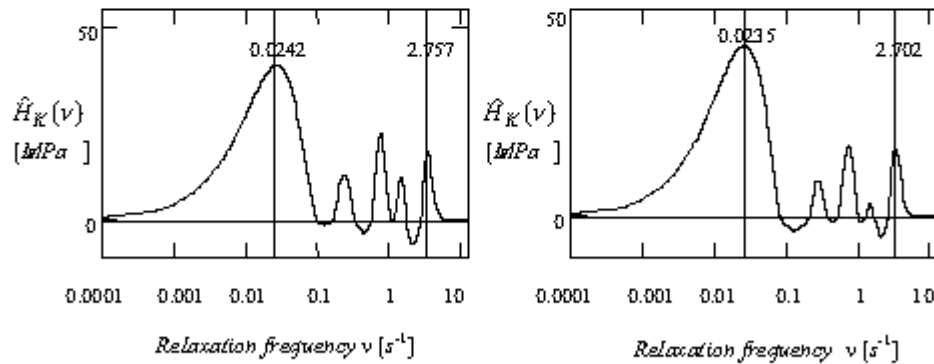


Fig. 4. The relaxation spectra models $\hat{H}_K(v)$ of two samples of beet sugar root

CONCLUSIONS

A robust algorithm has been found for the calculation of relaxation and retardation spectra from the measurement data of the linear relaxation modulus and creep compliance discrete-time measurements. The approach proposed is based on the approximation of the spectrum by finite linear combination of the basic Chebyshev functions. As a result, the primary infinite dimensional dynamic optimization problem of the continuous relaxation spectrum identification is reduced to the static linear-quadratic programming task. Tikhonov regularization and generalized cross validation are used to solve it, thus the stability of the resulting scheme is guaranteed. Due to the choice of the Chebyshev basic functions, for which the basic functions for relaxation modulus are given by the simple analytical formula, the errors of the approximate quadrature rules of known in the literature relaxation and retardation spectra identification schemes [Paulson i in. 2000] are avoided here. The above is of great importance in the context of ill-posed inverse problem. The choice of the orthogonal basic functions guarantees that smoothing of the regularized solution of the linear-quadratic problem ensures smoothing of the resulting relaxation spectrum model. The choice of the scaling-time factor in order to achieve a good fit of the model to the experiment data is discussed. An analysis of the model accuracy is conducted in the case corrupted by additive 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. The numerical experimental studies suggest that the scheme proposed can be successfully used within a satisfactory range of both viscoelastic solids and liquids.

REFERENCES

- Björck Å. 1996.: Numerical Methods for Least Squares Problems. SIAM, Philadelphia, PA.
- Bzowska-Bakalarz M. 1994.: Właściwości mechaniczne korzeni buraków cukrowych. Rozprawy Naukowe Akademii Rolniczej w Lublinie, 166.
- Elster C., Honerkamp J., Weese J. 1991.: Using regularization methods for the determination of relaxation and retardation spectra of polymeric liquids. *Rheological Acta*, 30(2), 161-174.
- Flory A., McKenna G. B. 2004.: Finite Step Rate Corrections in Stress Relaxation Experiments: A Comparison of Two Methods. *J. Mechanics of Time-Dependent Materials*, 8(1), 17-37.
- Golacki K. 2002.: Lepkosprężyste charakterystyki korzeni buraków cukrowych. *Acta Agrophysica*, 78, 37-49.
- Golacki K., Kołodziej P., Stankiewicz A., Stropek Z. 2003.: Sprawozdanie merytoryczne z realizacji projektu KBN nr 5P06P00619 pt. "Charakterystyka odporności mechanicznej buraków cukrowych w aspekcie spotykanych w praktyce obciążeń mechanicznych", s. 214.
- Heinz W. E., Martin H. 1996.: Regularization of Inverse Problems. Kluwer Academic Publishers, Dordrecht.
- Honerkamp J. 1989.: Ill-posed problems in rheology. *Rheol. Acta* 28, 363-371.
- Lebiediew N.N. 1957.: Funkcje specjalne i ich zastosowania. PWN, Warszawa.
- Ljung L. 1999.: System Identification: Theory for the User. Prentice-Hall, Englewood Cliffs New Jersey.
- Mańczak K., Nahorski Z. 1983.: Komputerowa identyfikacja obiektów dynamicznych. PWN, Warszawa.
- Orbey N., Dealy J. M. 1991.: Determination of the relaxation spectrum from oscillatory shear data. *J. Rheol.* 35(6), 1035-1049.
- Paulson K. S., Jouvavleva S., McLeod C. N. 2000.: Dielectric Relaxation Time Spectroscopy. *IEEE Trans. on Biomedical Engineering*, 47, 1510-1517.
- Stankiewicz A. 2007.: Identyfikacja spektrum relaksacji lepkoelastycznych materiałów roślinnych. Rozprawa doktorska, Akademia Rolnicza w Lublinie, Lublin.
- Syed Mustapha S.M.F.D., Phillips T.N., 2000.: A dynamic nonlinear regression method for the determination of the discrete relaxation spectrum. *Journal of Physics D: Applied Physics* 33(10), 1219-1229.
- Tikhonov A.N., Arsenin V.Y. 1977.: Solutions of Ill-posed Problems. John Wiley and Sons New York, USA.
- Tautenhahn U. 1994.: Error estimates for regularized solutions of nonlinear ill-posed problems, *Inverse Problems*, 10, 485-500.
- Varah J. M. 1983.: Pitfalls in the numerical solutions of linear ill-posed problems. *SIAM J. Sci. Statist. Comput.* 4 (2), 164-176.
- Zapas L. J., Phillips J. C. 1971.: Simple shearing flows in polyisobutylene solutions. *J. Res. Nat. Bur. Stds.* 75A (1), 33-40.

IDENTYFIKACJA SPEKTR RELAKSACJI I RETARDACJI LEPKOSPĘŻYSTYCH
MATERIAŁÓW ROŚLINNYCH Z WYKORZYSTANIEM FUNKCJI CZEBYSZEWA
CZĘŚĆ III. BADANIA NUMERYCZNE I PRZYKŁAD ZASTOSOWANIA

Streszczenie. W pierwszej części pracy zaproponowano algorytm optymalnej w sensie najmniejszej sumy kwadratów aproksymacji spektrum częstotliwości relaksacji skończoną sumą ortogonalnych funkcji Czebyszewa na podstawie zakłóconych pomiarów modułu relaksacji zgromadzonych w dziedzinie czasu. Teoretyczna analiza dokładności modelu, zbieżności algorytmu oraz wpływu założeń pomiarowych na wyznaczony model była przedmiotem drugiej części pracy. W tej pracy, przeprowadzając badania numeryczne dla spektrum relaksacji danego rozkładem Gaussa, wykazano poprawność i efektywność opracowanej metody identyfikacji. Przedstawiono wyniki badań numerycznych dla modelu symulacyjnego, a także wyznaczono spektrum relaksacji cylindrycznej próbki buraka cukrowego badanego w stanie jednoosiowego naprężenia.

Słowa kluczowe: Spektrum relaksacji, identyfikacja, regularyzacja, funkcje Czebyszewa