

The task of comparison solves by the method of the dynamic programming only for **voice-frequency part** of signal, **got** in the temporal window on the threshold level of parameter $\rho(T_1)$.

Conclusion. By the stated algorithm the programmatic system which can be applied for **estimation of declinations** of parameters of vocal signals as function of the psycho physiological state of a speaker is realized.

Bibliographical references

1. **Chugay A. A.** Elaboration and research of hardwares of analysis of speech for diagnostics of the emotional state of man-operator. Abstract of the **dissertation** doc. – Dnepropetrovsk, 1988.
2. **Fant G.** Acoustic theory of **speechformation**. – M. Science, 1964.- 284p.
3. **Sapojcov M. A.** Vocal signal in cybernetics and communication. – M. Svjazizdat. 1963. – 472 p.
4. **Carpov O. N.** Technology of construction of devices of speech recognition. Monograph. – Д., – 2001. – 190 p.
5. **Carpov O. N.** Calculable charts of presentation of functions of many variables in the classes of functions of **less** number of variables. Monograph. – Д., 2003. – 120 p.
6. **Carpov O.N., Gabovich A.G., Marchenko V.G., Choroshko V.A., Tcserbak L.N.** Computer technologies of recognition of vocal signals. Monograph. – К., 2005.– 138 p.
7. Pat. 773689, USSR, **MKY** G 10 L 1/02. Device for the selection of frequency of the **basic** tone /O. N. Carпов, E. L. **Nosenko**, A. A. Chugay / **Openings**. Inventions. –1980.– № 39.– 247 p.

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V. V. Romanuke

Khmelnytsky National University

OPTIMAL WLF EQUATION OVER EXPERIMENTAL VISCOSITY MEASUREMENTS BY FINITE SET OF FIXED TEMPERATURES

За критерієм мінімальної відстані у функціональному просторі $L_p [T_1; T_N]$ визначено оптимальну температурну залежність в'язкості полімеру у формі ВЛФ-рівняння за N вимірюваннями його в'язкості при N фіксованих температурах зі сегмента $[T_1; T_N]$. Повністю представлено розроблене програмне забезпечення у формі MATLAB-функції для знаходження оптимальної температурної залежності згідно з відповідними вхідними даними.

Ключові слова: полімер, в'язкість, температурна залежність, температура переходу у скловидну речовину, ВЛФ-рівняння, функціональний простір, мінімальна відстань, поліетилентерефталат.

По критерию минимального расстояния в функциональном пространстве $L_p [T_1; T_N]$ определена оптимальная температурная зависимость вязкости полимера в форме ВЛФ-уравнения по N измерениям его вязкости при N фиксированных температурах из сегмента $[T_1; T_N]$. Полностью представлено разработанное программное обеспечение в форме MATLAB-функции для нахождения оптимальной температурной зависимости согласно соответствующим входным данным.

Ключевые слова: полимер, вязкость, температурная зависимость, температура стеклования, ВЛФ-уравнение, функциональное пространство, минимальное расстояние, полиэтилентерефталат.

By the minimal distance criterion in the functional space $L_p [T_1; T_N]$ there has been determined the optimal temperature dependence of polymer viscosity in the WLF equation form over N measurements of its viscosity by N fixed temperatures from the segment $[T_1; T_N]$. There has been fully represented the designed software in the MATLAB-function form for finding the optimal temperature dependence in compliance with the corresponding input data.

Key words: polymer, viscosity, temperature dependence, glass transition temperature, WLF equation, functional space, minimal distance, polyethylene terephthalate.

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Introduction and problem raising. The Williams — Landel — Ferry equation (WLF equation) is a simple and simultaneously pretty exact formula for temperature dependence of polymer materials viscosity η [1; 2]. It actually works within the temperature segment $[T_g; T_g + 100]$ by the glass transition temperature T_g in Kelvin degrees [3], determined for the fixed polymer system. The WLF equation is

$$\eta(T) = \eta_g \cdot 10^{\frac{C_1(T-T_g)}{C_2+T-T_g}}, \quad (1)$$

for $T \in [T_g; T_g + 100]$ with the viscosity η_g measured by the temperature T_g , where C_1 and C_2 are constants being the functions of T_g . Obviously, that for obtaining the constants C_1 and C_2 it is sufficient to carry out the two viscosity measurements by the known T_g and η_g , what will give the system of two equations (1) with respect to the unknown C_1 and C_2 . However, the glass transition temperature may vary even for the same type of polymer material, depending on its vitrification speed and other operation factors. Besides, even if this temperature is fixed and learned, it is very uneasy to measure the polymer viscosity at T_g [4, 5]. That is why generally there is need to carry out the four polymer viscosity measurements

$$\{\eta_i\}_{i=1}^4 = \{\eta(T_i)\}_{i=1}^4 = \left\{ \eta_g \cdot 10^{\frac{C_1(T_i-T_g)}{C_2+T_i-T_g}} \right\}_{i=1}^4,$$

$$T_i \in (T_g; T_g + 100) \quad \forall i = \overline{1, 4}, \quad T_i < T_{i+1} \quad \forall i = \overline{1, 3} \quad (2)$$

for obtaining the constants C_1 and C_2 with also unknown T_g and η_g . But the problem is that the WLF equation (1) is still just an approximately rough model of real unknown temperature dependence $\eta = \eta(T)$, and for its as detailed as possible learning there is need to carry out the N polymer viscosity measurements

$$\{\eta_i\}_{i=1}^N = \{\eta(T_i)\}_{i=1}^N = \left\{ \eta_g \cdot 10^{\frac{C_1(T_i-T_g)}{C_2+T_i-T_g}} \right\}_{i=1}^N,$$

$$T_i \in (T_g; T_g + 100) \quad \forall i = \overline{1, N}, \quad T_i < T_{i+1} \quad \forall i = \overline{1, N-1}, \quad (3)$$

taking $N = 4$ and getting (2) at least. Those N measurements will give possibility to obtain $\frac{N!}{(N-4)! \cdot 4!}$ groups

$$\left\{ \left\{ \left\{ C_1(T_h, T_j, T_k, T_l), C_2(T_h, T_j, T_k, T_l), \dots \right. \right. \right. \\ \left. \left. \left. T_g(T_h, T_j, T_k, T_l), \eta_g(T_h, T_j, T_k, T_l) \right\}_{h=4}^N \right\}_{j=3}^{h-1} \right\}_{k=2}^{j-1} \right\}_{l=1}^{k-1} \quad (4)$$

of the constants C_1 and C_2 with T_g and η_g , what will allow to have

$\frac{N!}{(N-4)! \cdot 4!}$ different WLF equations

$$\left\{ \left\{ \left\{ \left\{ \eta_{ijkl}(T) \right\}_{h=4}^N \right\}_{j=3}^{h-1} \right\}_{k=2}^{j-1} \right\}_{l=1}^{k-1} = \\ = \left\{ \left\{ \left\{ \left\{ \eta_g(T_h, T_j, T_k, T_l) \cdot 10^{\frac{C_1(T_h, T_j, T_k, T_l)[T-T_g(T_h, T_j, T_k, T_l)]}{C_2(T_h, T_j, T_k, T_l)+T-T_g(T_h, T_j, T_k, T_l)}} \right\}_{h=4}^N \right\}_{j=3}^{h-1} \right\}_{k=2}^{j-1} \right\}_{l=1}^{k-1} \quad (5)$$

of the type (1). The stated problem core is how to select the most appropriate WLF equation

$$\eta_g(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*}) \cdot 10^{\frac{C_1(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})[T-T_g(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})]}{C_2(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})+T-T_g(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})}} = \\ = \eta_g^* \cdot 10^{\frac{C_1(T-T_g^*)}{C_2+T-T_g^*}} = \eta^*(T) \in \left\{ \left\{ \left\{ \left\{ \eta_{ijkl}(T) \right\}_{h=4}^N \right\}_{j=3}^{h-1} \right\}_{k=2}^{j-1} \right\}_{l=1}^{k-1} \quad (6)$$

from that $\frac{N!}{(N-4)! \cdot 4!}$ WLF equations multiplicity.

Analysis of investigations on polymer viscosity temperature dependence. Viscosity of polymer systems, which is measured by flow in shear, is the easiest for experimental study, and it is the most important in praxis amongst other mechanical polymer properties. To investigate the polymer viscosity temperature dependence $\eta = \eta(T)$ is very smart for comprehending the mechanism of its flow, including exploration of the macromolecular behavior by their deformations. Polymer viscosity temperature dependence influences strongly on the regime of the polymer recycling process, defining the quality and certain properties of the future re-polymer material. There are many investigators of polymer viscosity temperature dependence, where it ought to be underlined S. A. Arrhenius, Y. I. Frenkel, H. Eyring, A. Doolittle, M. L. Williams, R. F. Landel, J. D. Ferry, G. S. Fulcher, G. Tammann, W. Hesse, A. Kovacs, G. Gee, S. Ishihara, A. A. Miller, A. I. Bachinskiy, M. H. Cohen, D. Turnbull, F. Bueche, P. B. Macedo, T. A. Litovitz, R. B. Boyer, N. I. Shyshkin, V. G. Kulichikhin, R. S. Porter, J. F. Johnson, A. B. Bestul, H. V. Belcher, R. N. Haward, H. Breuer, G. Rehage, A. V. Tobolskiy, R. Simha, S. Krause, G. V. Vinogradov, A. Y. Malkin. The WLF equation (1) is connected with unconfined space conception [1, 2, 6] and it was grounded under that, though it is rather not the ideal model for polymer viscosity temperature dependence when the temperature is out of the segment $[T_g; T_g + 100]$. The unanswered question of optimal narrowing the WLF equations (5) multiplicity also originates with the issue of how to fix the N points $\{T_i\}_{i=1}^N$ within the interval $(T_g; T_g + 100)$, giving those $N!/((N-4)!4!)$ WLF equations.

Paper purpose and assignments. After having carried out the N polymer viscosity measurements (3), where $N \in \mathbb{N} \setminus \{1, 2, 3\}$, within the interval $(T_g; T_g + 100)$, here is the purpose to select the most appropriate WLF equation (6) amongst the $N!/((N-4)!4!)$ different WLF equations (5), obtained by the corresponding groups of four parameters (4). For this it should be applied the minimal functional distance criterion between each element of the set (5) and $(N-1)$ -linked polyline $\eta_0 = \eta_0(T)$, that in order links the points $[T_i \ \eta_i]$ та $[T_{i+1} \ \eta_{i+1}] \ \forall i = \overline{1, N-1}$. The base functional space, that is to be applied, is obviously defined within the band $[T_1; T_N]$.

Finding the optimal temperature dependence amongst the dependences (5). If look at the band $[T_1; T_N]$ of the plane \mathbb{R}^2 then the practically certain functional space, to be applied with its metric for comparing a couple of inner functional elements, is $L_p [T_1; T_N]$ for $p \geq 1$. In $L_p [T_1; T_N]$ the distance $\rho_{L_p [T_1; T_N]}(\eta_{ijkl}(T), \eta_0(T))$ between the polymer viscosity temperature dependence $\eta_{ijkl}(T)$ and polyline $\eta_0(T)$ is the norm of their difference $\eta_{ijkl}(T) - \eta_0(T)$, that is

$$\rho_{L_p [T_1; T_N]}(\eta_{ijkl}(T), \eta_0(T)) = \left(\int_{T_1}^{T_N} |\eta_{ijkl}(T) - \eta_0(T)|^p dT \right)^{\frac{1}{p}},$$

$$h = \overline{4, N}, \quad j = \overline{3, h-1}, \quad k = \overline{2, j-1}, \quad l = \overline{1, k-1}. \quad (7)$$

Into (7) we substitute $\eta_{ijkl}(T)$ with the element from (5), and the polyline

$$\eta_0(T) = \alpha_{i+1,i} + \beta_{i+1,i} T \quad \text{by } T \in [T_i; T_{i+1}] \quad \forall i = \overline{1, N-1}, \quad (8)$$

where

$$\alpha_{i+1,i} = \eta_i - T_i \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}} \quad \forall i = \overline{1, N-1} \quad (9)$$

and

$$\beta_{i+1,i} = \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}} \quad \forall i = \overline{1, N-1}. \quad (10)$$

Going further, take (5) explicitly with (8) — (10), and the distance (7) turns into

$$\rho_{L_p [T_1; T_N]}(\eta_{ijkl}(T), \eta_0(T)) = \left(\sum_{i=1}^{N-1} \int_{T_i}^{T_{i+1}} |\eta_{ijkl}(T) - \eta_0(T)|^p dT \right)^{\frac{1}{p}} =$$

$$= \left(\sum_{i=1}^{N-1} \int_{T_i}^{T_{i+1}} \eta_g(T_h, T_j, T_k, T_l) \cdot 10^{\frac{C_1(T_h, T_j, T_k, T_l)[T - T_g(T_h, T_j, T_k, T_l)]}{C_2(T_h, T_j, T_k, T_l) + T - T_g(T_h, T_j, T_k, T_l)}} - \right.$$

$$\left. - \eta_i + T_i \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}} - \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}} T \right)^{\frac{1}{p}} dt$$

$$= \left(\sum_{i=1}^{N-1} \int_{T_i}^{T_{i+1}} \eta_g(T_h, T_j, T_k, T_l) \cdot 10^{\frac{C_1(T_h, T_j, T_k, T_l)[T - T_g(T_h, T_j, T_k, T_l)]}{C_2(T_h, T_j, T_k, T_l) + T - T_g(T_h, T_j, T_k, T_l)}} + \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}}(T_i - T) - \eta_i \left| dT \right|^{\frac{1}{p}} \right)^p, \quad h = \overline{4, N}, \quad j = \overline{3, h-1}, \quad k = \overline{2, j-1}, \quad l = \overline{1, k-1}. \quad (11)$$

Consequently, the optimal WLF equation (6) amongst the $\frac{N!}{(N-4)! \cdot 4!}$

different WLF equations (5) is determined as

$$\eta^*(T) \in \arg \min_{\substack{\eta_{ijkl}(T) \\ h=\overline{4, N} \\ j=\overline{3, h-1} \\ k=\overline{2, j-1} \\ l=\overline{1, k-1}}} \rho_{\mathbb{L}_p[T_1; T_N]}(\eta_{ijkl}(T), \eta_0(T)) = \min_{\substack{\eta_{ijkl}(T) \\ h=\overline{4, N} \\ j=\overline{3, h-1} \\ k=\overline{2, j-1} \\ l=\overline{1, k-1}}} \left\{ \left(\sum_{i=1}^{N-1} \int_{T_i}^{T_{i+1}} \eta_g(T_h, T_j, T_k, T_l) \cdot 10^{\frac{C_1(T_h, T_j, T_k, T_l)[T - T_g(T_h, T_j, T_k, T_l)]}{C_2(T_h, T_j, T_k, T_l) + T - T_g(T_h, T_j, T_k, T_l)}} + \frac{\eta_i - \eta_{i+1}}{T_i - T_{i+1}}(T_i - T) - \eta_i \left| dT \right|^{\frac{1}{p}} \right)^p \right\} \quad (12)$$

by the minimal functional distance criterion in the space $\mathbb{L}_p[T_1; T_N]$.

For finding the optimal WLF dependence $\eta^*(T)$ it is preferable to use the technical computing environment MATLAB. Firstly there should be solved each of the $\frac{N!}{(N-4)! \cdot 4!}$ systems of the four nonlinear equations

$$\eta_h - \eta_g \cdot 10^{\frac{C_1(T_h - T_g)}{C_2 + T_h - T_g}} = 0, \quad h = \overline{4, N}, \quad (13)$$

$$\eta_j - \eta_g \cdot 10^{\frac{C_1(T_j - T_g)}{C_2 + T_j - T_g}} = 0, \quad j = \overline{3, h-1}, \quad (14)$$

$$\eta_k - \eta_g \cdot 10^{\frac{C_1(T_k - T_g)}{C_2 + T_k - T_g}} = 0, \quad k = \overline{2, j-1}, \quad (15)$$

$$\eta_l - \eta_g \cdot 10^{\frac{C_1(T_l - T_g)}{C_2 + T_l - T_g}} = 0, \quad l = \overline{1, k-1}, \quad (16)$$

with respect to the four unknown parameters $C_1(T_h, T_j, T_k, T_l)$, $C_2(T_h, T_j, T_k, T_l)$, $T_g(T_h, T_j, T_k, T_l)$, $\eta_g(T_h, T_j, T_k, T_l)$, where the s -th system is solved by the fixed $h \in \{\overline{4, N}\}$, $j \in \{\overline{3, h-1}\}$, $k \in \{\overline{2, j-1}\}$ and $l \in \{\overline{1, k-1}\}$, $s = 1, \frac{N!}{(N-4)! \cdot 4!}$. The system (13) — (16) may be

numerically solved, using the MATLAB solver of systems of nonlinear equations of several variables (figure 1).

When the $\frac{N!}{(N-4)! \cdot 4!}$ systems (13) — (16) are solved, it remains to compute (11), integrating numerically, and find such function (6), that allows (11) to stay the most minimal. Parameters $C_1^* = C_1(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})$, $C_2^* = C_2(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})$, $T_g^* = T_g(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})$ and $\eta_g^* = \eta_g(T_{h^*}, T_{j^*}, T_{k^*}, T_{l^*})$ of this function may be considered as the most appropriate for the given polymer material. And the temperatures T_{h^*} , T_{j^*} , T_{k^*} and T_{l^*} should be regarded as the basic points for measuring the given polymer class viscosity.

As an example there are the five viscosity measurements

$$\{\eta_i\}_{i=1}^5 = \{133.8, 69.9, 37.5, 21.3, 12.9\} \quad (17)$$

of the polyethylene terephthalate (Dacron) [7, 8], carried out by the temperatures

$$\{T_i\}_{i=1}^5 = \{403.05, 412.15, 422.15, 432.05, 442.05\} \quad (18)$$

with the Brookfield viscometer CAP2000+ (figure 2). As it is known, the polyethylene terephthalate glass transition temperature lies between 67 and 81 Celsius degrees, where accordingly the amorphous polyethylene

terephthalate has $T_g \approx 340.15$ K, and crystalline polyethylene terephthalate has $T_g \approx 354.15$ K. Then, theoretically, temperatures $\{T_i\}_{i=1}^4$ from (18) belong to the segment $[T_g; T_g + 100]$ by $T_g \in [340.15; 354.15]$. Moreover, if the being recycled polymer has been crumbled up, the glass transition temperature of such deformed polymer becomes lower. Nevertheless, the sentenced above polyethylene terephthalate glass transition temperatures are just averaged evaluations, which may vary broadly. Hence the temperature set (18) here may be considered as the practical example for demonstrating the developed MATLAB software in accomplishing (12).

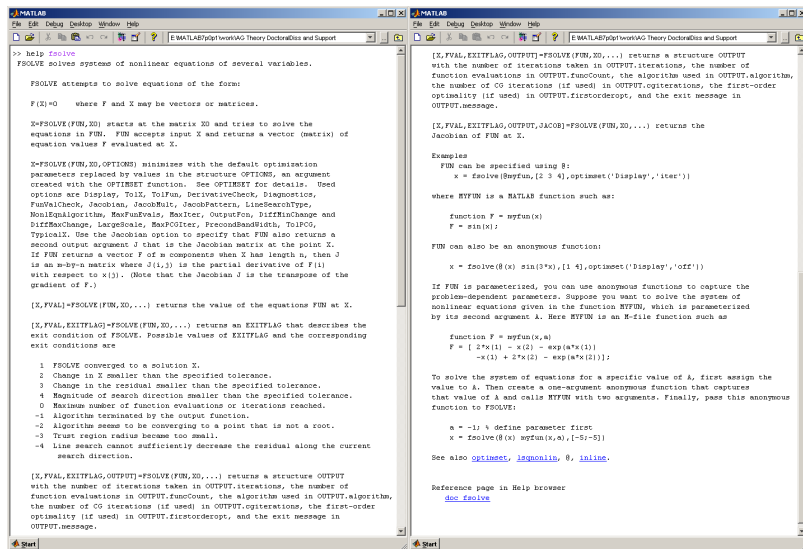


Fig. 1. MATLAB Command Window: the call for help on MATLAB solver of systems of nonlinear equations of several variables, named «fsolve»

CAP 1000+ & CAP 2000+ Cone & Plate Viscometers



BROOKFIELD VISCOMETERS
 T: 800.628.8139 or 508.946.6200 F: 508.946.6262 www.brookfieldengineering.com

MODEL	SPEEDS		number of beakers
	Min.	Max.	
CAP 1000+	0.01	300/750	2
CAP 2000+	0.01	5-1K	995

*Dependent on cone selected
 M=1.0mm H=1.0mmax 0.1-Complete w/Probe+M8SpareBeakers

Fig. 2. Brookfield viscometer CAP2000+ and some its characteristics [9]

The $\frac{N!}{(N-4)!4!}$ systems (13) — (16) solver code «wlf_eval» has been

screenshot into figure 3, where it was laid $N=5$. This code uses beforehand saved mat-file, named «viscosity01», and containing the sets (17) and (18). Also there is used the subfunction «four_wlf_eq». After having run and accomplished this code, there are saved $\frac{N!}{(N-4)!4!}$ mat-

files with the found numerically unknown parameters in (4). These files will be loaded within the main code, developed as a MATLAB-function «opt_wlf» (figure 4), working with other MATLAB-function «line2points» (figure 5) for obtaining the line (8) constants (9) and (10).

```

1 function [x_star] = wlf_eval
2   % N=5
3   for k4=1:5
4     for k3=3:k4-1
5       for k2=2:k3-1
6         for k1=1:k2-1
7           save wlf_4points_k k1 k2 k3 k4
8           x0 = [-5; 100; 10000; 360]; % Make a starting guess at the solution
9           %options = optimset('Display','iter','MaxFunEvals',900,'MaxIter',250); % Option to display output
10          options = optimset('MaxFunEvals',9000,'MaxIter',2500); % Option to display output
11          [k1 k2 k3 k4]
12          [x_star, fval] = fsolve(@four_wlf_eq, x0, options) % Call optimizer
13          eval(['K1=' num2str(x_star(1)) ''])
14          eval(['eta_g=' num2str(x_star(2)) ''])
15          eval(['Tg=' num2str(x_star(3)) ''])
16          eval(['eta_g_Tg=' num2str(x_star(4)) ''])
17          eval(['save wlf_4points_' num2str(k1) num2str(k2) num2str(k3) num2str(k4) ' K1 K2 eta_g Tg'])
18        end
19      end
20    end
21  end
22
23 function F = four_wlf_eq(x)
24 load viscosity01
25 temperature = temperature + 273.15;
26 load wlf_4points_k
27 F = [viscosity(k1) - x(3)*10^(x(1)*(temperature(k1) - x(4))/(x(2) + temperature(k1) - x(4)));
28      viscosity(k2) - x(3)*10^(x(1)*(temperature(k2) - x(4))/(x(2) + temperature(k2) - x(4)));
29      viscosity(k3) - x(3)*10^(x(1)*(temperature(k3) - x(4))/(x(2) + temperature(k3) - x(4)));
30      viscosity(k4) - x(3)*10^(x(1)*(temperature(k4) - x(4))/(x(2) + temperature(k4) - x(4)))];
```

Fig. 3. The systems (13) — (16) solver code, that may be run as from the MATLAB Command Window line, as well as just pressing F5 key

```

1 function [K1_star K2_star eta_g_star Tg_star h_star_k_star_l_star distance_wlf] = opt_wlf (Temperature_Set, Viscosity_Set, p)
2 if nargin < 3
3   p = 2;
4 end
5 c = 0;
6 for j=2:length(Temperature_Set)
7   for l=1:j-1
8     [beta alpha] = line2points (Temperature_Set(j), Viscosity_Set(j), Temperature_Set(l), Viscosity_Set(l), 0);
9     eval(['beta=' num2str(beta) 'alpha=' num2str(alpha) '']);
10    eval(['alpha=' num2str(alpha) 'beta=' num2str(beta) '']);
11    c=c+1;
12  end
13  distance_wlf = 0; u = 0;
14  for h=1:5
15    for j=3:h-1
16      for k=2:j-1
17        for l=1:k-1
18          eval(['load wlf_4points_' num2str(l) num2str(k) num2str(j) num2str(h)'])
19          c = 1; distance_p = 0;
20          while c < length(Temperature_Set)
21            eval(['beta=' num2str(beta) 'alpha=' num2str(alpha) '']);
22            eval(['alpha=' num2str(alpha) 'beta=' num2str(beta) '']);
23            eta_wlf = eta_g*10.^((K1*(Temperature_Set(c)+0.0001:Temperature_Set(c+1) - 0.0001)-Tg) ./ ...
24              (K2+(Temperature_Set(c)+0.0001:Temperature_Set(c+1) - 0.0001)-Tg));
25            line = beta*(Temperature_Set(c)+0.0001:Temperature_Set(c+1) - 0.0001) + alpha;
26            distance_p(c) = sum((eta_wlf - line).^p)*0.0001;
27            c = c + 1;
28          end
29          u = u + 1;
30          distance_wlf(u, 1) = (sum(distance_p))^(1/p); distance_wlf(u, 2:5) = [h j k l];
31          eval(['distance_' num2str(h) num2str(j) num2str(k) num2str(l) '=distance_wlf(u, 1)']);
32        end
33      end
34    end
35  end
36 end
37 h_star_k_star_l_star = distance_wlf(find(distance_wlf == min(distance_wlf(:, 1)), 2:5);
38 eval(['load wlf_4points_' num2str(h_star_k_star_l_star(4)) num2str(h_star_k_star_l_star(3)) ...
39       num2str(h_star_k_star_l_star(2)) num2str(h_star_k_star_l_star(1))]);
40 K1_star = K1; K2_star = K2; eta_g_star = eta_g; Tg_star = Tg;
```

Fig. 4. MATLAB-function «opt_wlf» code for completing the optimal WLF equation (12) determination

```

1 function [beta alpha] = line2points(x1, y1, x2, y2, equation_display)
2 % It returns the coefficients of the line, passing through the two points [x1 y1] and [x2 y2].
3 % Also it returns the equation of the line if needed and been checked in the input.
4 if nargin == 4
5   equation_display = 0;
6 end
7 if x1 == x2
8   beta = []; alpha = [];
9   if equation_display == 0
10    disp([' The equation of the line, passing through the two points [' num2str(x1) ' ' num2str(y1) ' and [' num2str(x2) ' ' num2str(y2) '], is'])
11    disp([' x = ' num2str(x1)])
12  end
13  return
14 end
15 beta = (y1 - y2)/(x1 - x2);
16 alpha = y1 - x1*(y1 - y2)/(x1 - x2);
17 if equation_display == 0
18   disp([' The equation of the line, passing through the two points [' num2str(x1) ' ' num2str(y1) ' and [' num2str(x2) ' ' num2str(y2) '], is'])
19   if beta == 0
20     disp([' y = ' num2str(alpha)])
21   else
22     if alpha < 0
23       disp([' y = ' num2str(beta) ' x - ' num2str(abs(alpha))])
24     else
25       if alpha == 0
26         disp([' y = ' num2str(beta) ' x'])
27       else
28         disp([' y = ' num2str(beta) ' x + ' num2str(alpha)])
29       end
30     end
31   end
32 end
```

Fig. 5. MATLAB-function «line2points» code, used as a subfunction within MATLAB-function «opt_wlf» for obtaining the line (8) constants (9) and (10)

The saved results with evaluated five groups (4) are shown on figure 6. As it is seen, here has been obtained even greater polyethylene terephthalate glass transition temperature, than expected before running the systems (13) — (16) solver.

Group	Maximum number of function increase options.MaxFunEvals	x_star	fval	K1	K2	eta_g	Tg
1	1.0e+003	1.0e+003 + -0.0065 0.1014 9.2951 0.3630	-0.0101 -0.0188 0.2041 -0.2275	-6.5069	101.4483	2.2551e+003	362.9992
2	1.0e+003	1.0e+003 + -0.0065 0.1009 9.2467 0.3631	-0.0128 -0.0252 0.1860 -0.2612	-6.4861	100.9108	9.2667e+003	363.0736
3	1.0e+003	1.0e+003 + -0.0065 0.1011 9.1871 0.3633	-0.0537 0.1536 -0.0833 -0.1298	-6.5040	101.1321	9.1871e+003	363.2563
4	1.0e+003	1.0e+003 + -0.0065 0.1008 9.2684 0.3632	-0.0274 0.2757 -0.1329 -0.2070	-6.4893	100.7819	9.2684e+003	363.1510
5	1.0e+004	1.0e+004 + -0.0007 0.0101 1.0397 0.0362	-0.0811 0.2794 -0.1329 -0.1529	-6.5652	100.5348	1.0397e+004	362.4530

Fig. 6. Five groups (4) of the evaluated parameters C_1 and C_2 with T_g and η_g in WLF equation

The result of the function «opt_wlf» run has been screenshot into figure 7, whereupon

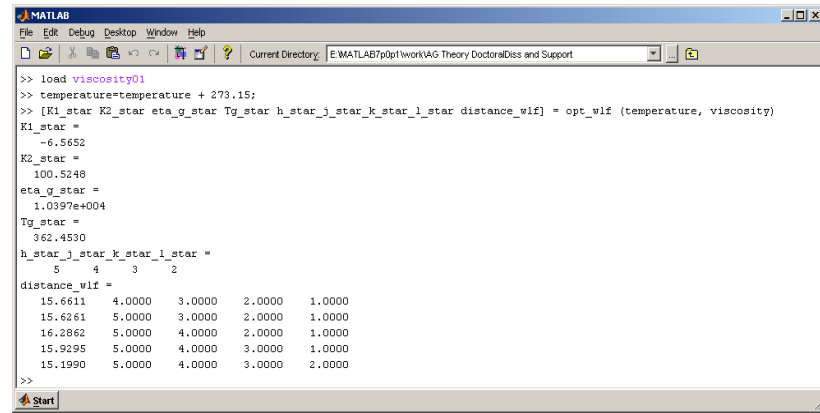


Fig. 7. The most appropriate WLF equation (6) by the criterion (12)

$$\begin{aligned} \eta^*(T) &= \eta_{5432}(T) = \\ &= \eta_g(T_5, T_4, T_3, T_2) \cdot 10^{\frac{C_1(T_5, T_4, T_3, T_2)[T - T_g(T_5, T_4, T_3, T_2)]}{C_2(T_5, T_4, T_3, T_2) + T - T_g(T_5, T_4, T_3, T_2)}} = \\ &= \eta_g^* \cdot 10^{\frac{C_1^*(T - T_g^*)}{C_2^* + T - T_g^*}} = 10396.6651 \cdot 10^{\frac{-6.5652(T - 362.453)}{100.5248 + T - 362.453}} \end{aligned} \quad (19)$$

within the segment

$$[T_g^*; T_g^* + 100] = [362.453; 462.453],$$

involving the set (18). The optimal WLF equation (19) has been obtained by the criterion (12) in the space $\mathbb{L}_2[403.05; 442.05]$ and holds the points

$$\begin{aligned} [T_5 \quad \eta_5] &= [442.05 \quad 12.9], \\ [T_4 \quad \eta_4] &= [432.05 \quad 21.3], \\ [T_3 \quad \eta_3] &= [422.15 \quad 37.5] \end{aligned}$$

and

$$[T_2 \quad \eta_2] = [412.15 \quad 69.9]$$

of the band $[403.05; 442.05]$ on the plane \mathbb{R}^2 . The optimal WLF equation (19) with four-linked polyline $\eta_0(T)$ is visualized on figure 8.

And now it is the phase to make conclusions on the applied WLF equation optimality criterion and on the developed software application domain.

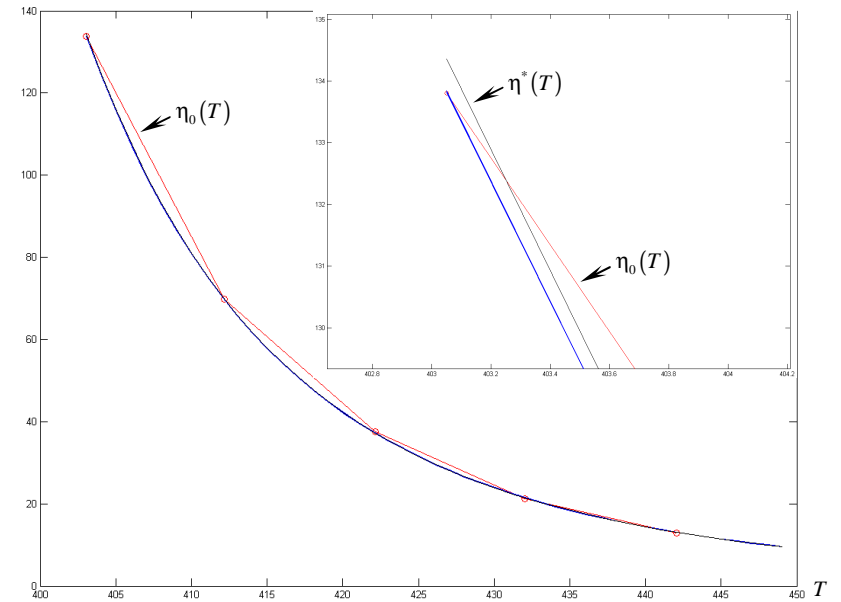


Fig. 8. The optimal WLF equation (19) with four-linked polyline $\eta_0(T)$ for the five viscosity measurements (17) by the set of fixed temperatures (18)

Conclusions and perspective for further investigation. The developed MATLAB-function «opt_wlf», co-working with MATLAB-subfunction «line2points» after having acquired the solver «wlf_eval» data (4), allows to determine numerically the optimal WLF equation $\eta^*(T)$ for figuring the given polymer viscosity temperature dependence within the segment $[T_g^*; T_g^* + 100]$ by $T_g^* = T_g(T_h^*, T_j^*, T_k^*, T_l^*)$ in (6). Except C_1^* , C_2^* , η_g^* and T_g^* , into MATLAB Workspace there are returned the most appropriate numbers h^* , j^* , k^* , l^* of the measurements (3), and all the distances (11). Surely, the been applied criterion of minimal functional distance in the space $\mathbb{L}_p[T_1; T_N]$ is not the perfect, as it is grounded on some practical suggestions. The obtained parameters C_1^* , C_2^* , η_g^* and T_g^* of the most appropriate WLF equation $\eta^*(T)$ for the given polymer viscosity measurements may be automatically used for calculating the viscosity of this polymer in any point of the segment $[T_g^*; T_g^* + 100]$, that

includes also $[T_1; T_N]$. This will be applied for correct and rationalized selection of regime in the polymer recycling [10, 11], where the viscosity sensibility to the temperature change is determinative. Admittedly, the criterion of selecting optimally the WLF equation (1) does not answers the question on how many measurements N one should do for a polymer within the given temperature range. Also it does not speak whether the given number N is sufficient or not. These things are the subject for further investigation of the temperature dependence of polymer materials viscosity in the WLF equation form.

Bibliographical references

12. Williams M. L. The temperature dependence of relaxation mechanisms in amorphous polymers and other glass-forming liquids / M. L. Williams, R. F. Landel, J. D. Ferry // J. Am. Chem. Soc. – 1955. – V. 77, N. 14. – P. 3701 – 3707.
13. Виноградов Г. В. Реология полимеров / Г. В. Виноградов, А. Я. Малкин. – М., 1977. – 440 с.
14. http://en.wikipedia.org/wiki/Glass_transition_temperature
15. Малкин А. Я. Диффузия и вязкость полимеров. Методы измерения / А. Я. Малкин, А. Е. Чалых. – М., 1979. – 304 с.
16. Фогельсон Р. Л. Температурная зависимость вязкости / Р. Л. Фогельсон, Е. Р. Лихачев // Журнал технической физики. – 2001. – Т. 71, вып. 8. – С. 128 – 131.
17. http://en.wikipedia.org/wiki/Temperature_dependence_of_liquid_viscosity
18. <http://www.europrint-ua.com/pet-features.html>
19. http://www.ekoresurs.ru/pet__polietilenterftal
20. <http://www.brookfieldengineering.com>
21. <http://en.wikipedia.org/wiki/Polymer>
22. <http://www.recyclers.ru/modules/section/category.php?categoryid=17>

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І. В. Дроздова¹, М. Г. Сидорова², О. О. Харченко¹,
С. В. Романенко¹, С. Л. Поріц¹, Г. Б. Чумак³

¹ Український Державний науково-дослідний інститут медико-соціальних проблем інвалідності, м. Дніпропетровськ

² Дніпропетровський національний університет імені Олеся Гончара

³ Санаторій «Зорі України», м. Ялта

ІНФОРМАЦІЙНА ТЕХНОЛОГІЯ ДІАГНОСТИКИ ХРОНІЧНОЇ СЕРЦЕВОЇ НЕДОСТАТНОСТІ

Запропоновано обчислювальну технологію кластерного аналізу даних ехокардіографічного обстеження хворих на хронічну серцеву недостатність, що забезпечує відбір інформативних ознак, оцінку якості розбиття, підтримку прийняття рішень, встановлення меж «норма-патологія».

Ключові слова: інформативні ознаки, кластерний аналіз, якість розбиття, прийняття рішень, нормальний розподіл, межі «норма-патологія».

Предложена вычислительная технология кластерного анализа данных эхокардиографии у больных с хронической сердечной недостаточностью, которая обеспечивает отбор информативных признаков, оценку качества разделения, поддержку принятия решений, определение границ «норма-патология».

Ключевые слова: информативные признаки, кластерный анализ, качество разделения, принятие решений, границы «норма-патология».

The computing technology of cluster analysis of echocardiography data's in patients with chronic heart failure was proposed. The method provides selection of informative signs, evaluation of differences quality, supports to take decisions, determination between «norm» and «pathology» limits.

Key words: informative signs, cluster analysis, evaluation of differences quality, taking a decision, normal distribution, «norm» and «pathology» limits.

Вступ. Хронічна серцева недостатність із систолічною дисфункцією (ХСН) – це симптомокомплекс, що супроводжується такими ознаками, як задишка у спокої та під час фізичного навантаження, хрипи в легенях і набряк гомілок, при наявності об'єктивних доказів патологічних змін міокарду або функцій серця у спокої [1; 2; 3]. Поширеність ХСН у популяції коливається від 2 до 3 %, а серед осіб віком 70–80 років сягає 10–20 %; 50 % пацієнтів

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