

ALGORITHM FOR COMPUTER PROCESSING OF KINETIC DEPENDENCES OF THE RESPONSE OF A GAS SENSOR WITH INTELLIGENT COMPONENTS

Abstract. The purpose of the work is to develop an algorithm using intelligent components that will allow processing of experimental data of response kinetics of resistive gas sensors based on the algorithm of the model of the stretched exponential function of Kohlrausch Williams Watts, without operator intervention. The problems of implementing full automation of the information measuring system for the study of the main characteristics of gas sensitive sensors the selection of the most informative time interval are describe. The algorithm for processing the experimental kinetic dependence of the response of gas sensors based on the model of a stretched exponential function with intelligent components that allow choosing the most informative time interval from the processed kinetic dependences is present.

Keywords: algorithm, stretched exponential function, gas sensor, response, parameter calculation, automation, information and measurement system.

Introduction. The study of the kinetic dependences of the gas sensitivity of gas sensor materials allows us to obtain more accurate and detailed information about their characteristics, which is important in their search and practical use [1-3]. These dependencies are also of interest for monitoring finished gas sensors.

In practice, such measurements are fraught with some difficulties. This process usually takes a long time and requires multiple cycles of processing and analysis of large amounts of experimental data. To eliminate routine operations associated with the processing of experimental data, to increase the speed, accuracy and information content of the research process itself, it seems relevant to automate it using computer technology. In [4, 5] the prospects for solving such a problem by creating a specialized information and measurement system (IMS) are shown.

It should be note that one of the key components of the software of such IMS is the algorithmization of experimental data processing processes based on appropriate mathematical models [6-9]. For primary processing of data obtained from studies of gas sensors in [1, 4, 5], a phenomenological relaxation model is used based on the stretched exponential function Kohlrausch–Williams–Watts (KWW)

$f(t)=\exp[-(t/\tau)^\beta]$, where t - time, β and τ – parameters [10, 11]. It use to describe the kinetics of relaxation dependences of the response, in particular, at the stage of restoration of the gas sensitivity of the sensor.

As shown in [1], the use of this approach allows us to obtain significantly more information about the phenomena that determine the phenomenon of gas sensitivity of sensor materials. The data presented in [4] indicate the reality and effectiveness of computer processing of a significant amount of data in the process of carrying out the physical and chemical measurements under consideration.

However, the data processing algorithm used in this work does not allow the implementation of complete automation of the IMS for studying the main characteristics of gas-sensitive sensors. The main reason for this is the need to select a segment from the time dependence of the main parameter - sensitivity to the active gas, the data of which allows one to correctly estimate the parameter β of the KWW function, which approximates the kinetics of sensor recovery. These actions require the operator's direct participation in the data processing process. It should be note that in [12] an algorithm is proposed that makes it possible to exclude the participation of the operator in the process of processing and primary analysis of response kinetics measurement data. However, in this method, the value of the amplitude parameter S_0 of such a stretched exponential function must be determined independently, which is not always possible.

As is known, one of the rapidly developing areas of ensuring the automation of computer processing of measurements is the use of artificial intelligence tools and methods [13]. These methods are used in systems for monitoring the physical properties of various materials [14, 15], measuring mechanical quantities (aircraft positions) [16, 17], testing and analyzing faults of electronic devices [18], etc.

In this paper, an algorithm based on a stretched exponential function with intelligence components is proposed and justified, which makes it possible to exclude the participation of the operator in the process of processing and primary analysis of measurement data of the response kinetics of resistive gas sensors.

Description of the algorithm. As already indicated, the advantage of the algorithm for processing and primary data analysis used in [1, 4, 5] is the absence of any additional assumptions. Only the results of measurements of the kinetic dependence of the sensor response $S(t)$ are used. Accordingly, the approximating dependence used as a model for the primary phenomenological analysis of the experimental kinetic dependences of the response of a gas-sensitive sensor in the area after removal of the active gas was assume to be represented in the form

$$S(t) = S_0 \cdot \exp\left[-(t/\tau)^\beta\right]. \quad (1)$$

In accordance with [1, 19], the mathematical procedure for finding the value of the unknown coefficient β includes the following operations:

- numerical determination of the derivatives $d \log S(t) / dt$ based on the experimental kinetic dependence of the form (Fig. 1) and representation of this dependence in coordinates $t \times [d \log S(t) / dt]$ and $\log S(t)$;
- visual selection of the area above the specified dependence, where the accepted model is applicable (i.e., the dependence becomes straight, and the coefficient β itself is the tangent of its angle) and calculation of the value

$$\beta = \Delta \{ t \times [d \log S(t) / dt] / \Delta \log S(t); \quad (2)$$

Representation of the initial kinetic dependence in the selected area in coordinates $\ln S(t)$ and t^β (β - already known) and approximation of this dependence by a straight line allows you to determine the values of the remaining parameters of the KWW function using the following formulas

$$\tau = [-\Delta \ln S(t) / \Delta (t^\beta)]^{-1/\beta}; \quad S_0 = \exp\{\ln S(t) + (t/\tau)^\beta\}. \quad (3)$$

The disadvantages of the algorithm under consideration, such as significant errors associated with the operation of numerical differentiation, the need to support the data processing process by a qualified operator when choosing the most informative time interval in the experimental kinetic dependence. One of the possible means of overcoming shortcomings, as well as in selecting analytical expressions that describe the dependence of these parameters on the influence of one or another factor specified by the research program, seems to be the use of components of methods that are known for solving artificial intelligence problems [20, 21].

Below it is proposed to use this approach to determine the parameters of the KWW function that approximates the experimental kinetic dependence and their dependence on one or another factor x . This algorithm eliminates the need for operator participation in the process of analyzing intermediate data.

A description of the main operations of the algorithm under consideration can be present as follows.

1. The entire time range of each (i-th) experimental dependence $S(t)$ is divided into several intervals with a sufficient number of points for the numerical determination of the time derivative (for example, $n=4$).

2. These intervals are considered independent and are used to calculate several (n) sets of values for each of the parameters of the approximating KWW function (β , S_0 , τ). These sets can be presented in the form of tables $\{\beta_{k,j}\}$, $\{S_{0,k,j}\}$ и $\{\tau_{k,j}\}$. Index k corresponds to the number of the factor value, the influence of which is study in this experiment (for example, temperature T). This index varies from 0 to $(m-1)$, where m is the number of processed dependencies corresponding to different factor values. Index j is the number of the selected time segment of the relaxation dependence. $j=0, 1, \dots, n-1$ (in the example given $n=4$), $k=0, 1, \dots, m-1$ ($m=5$).

It should be noted that the parameter values (β , S_0 , τ), found in different time intervals have some scatter, the presence of which can be associated with the influence of both a random factor and the general degree of approximation of the description of relaxation processes of this type using the KWW function.

Based on the data from each interval of the experimental relaxation dependence, the coefficients of the approximating expression of the form (1) were determined using the well-known least squares method [22].

The measure of the quality of the approximation was the root-mean-square error of the approximation, divided by the empirical average value (coefficient of variation), which is determined for each section of the relaxation dependence using the formula

$$v_{k,j} = \frac{\sqrt{\sum_{i=0}^{N_k-1} [S_k^i - S_{0,k,j} \cdot \exp[-(t_k^i / \tau_{k,j})]]^2 / (N_k - 1)}}{\sum_{i=0}^{N_k-1} S_k^i / N_k} \quad (4)$$

where t_k^i and S_k^i - are the time and response values for the j -th section of the k -th kinetic dependence (at the value of the operating measurement factor x_k . N_k - is the number of experimental points of the k -th kinetic dependence.

To select the optimal section of each relaxation dependence, the condition of minimum value of the corresponding root-mean-square error of approximation was used, that is, the rule, which for the k -th kinetic dependence has the form

$$\text{IF } v_{k,jm} = \min(v_{k,j}), \text{ THEN the } jm\text{-th set of parameter values is selected. (5)}$$

It should be noted that to improve the quality of approximation, the size and location of the selected optimal area can be changed using other logical algorithms (for example, they can be expanded or shifted).

The numerical values of the parameters β_k , $S0_k$ and τ_k selected in this way are used to analyze their dependence on the influence of the variable operating measurement factor x .

3. The choice of the type of formulas that analytically represent the dependencies $\beta(x)$, $S0(x)$ and $\tau(x)$, can be based on dividing them into two most general classes: monotonic (decreasing or increasing) and having an extremum. It was assumed that in the studied range of factor values, monotonic ones can be approximately described by the simplest regression equations of the form

$$\beta_1(x, a0, a1) = a0 + a1, \quad (6)$$

$$\beta_1(x, a0, a1, a2) = a0 + a1 \cdot x + a2 \cdot x^2, \quad (7)$$

and those having an extremum - by the formula

$$\beta_3(x, a0, a1, a2) = a1 \cdot \exp\left[-\frac{(x-a1)^2}{2 \cdot a3^2}\right], \quad (8)$$

If necessary, a number of approximating functions can be expand and change. For the parameters of the KWW function parameters $S0$, τ you can also use similar approximations and procedures for their determination.

The values of the coefficients $a0$, $a1$ and $a2$ found by the least squares method, i.e. by minimizing the function

$$F_l(a1, a2, a3) = \sum_{k=0}^{n-1} [\beta_k - \beta_l(x_k, a0, a1, a2)]^2, \quad (9)$$

where $l=1,2,3$.

Analysis of the optimal use of approximating expressions (6)-(8) can be carried out on the basis of calculating the corresponding coefficients of variation $av_l^{(z)}$ using formulas similar to expression (4). The notation z takes the values β , $S0$ and τ , respectively.

The justification for the final choice of the type of approximating formula thus made in accordance with the simplest production rules of the form (3):

$$\text{IF } v_{lm}^{(z)} = \min(v_l^{(z)}), \text{ THEN the } lm\text{-th approximating formula selected.} \quad (10)$$

Test results. An example of the experimental kinetic dependence of the response at the stage of restoration of a resistive gas sensor sample shown in Fig. 1.

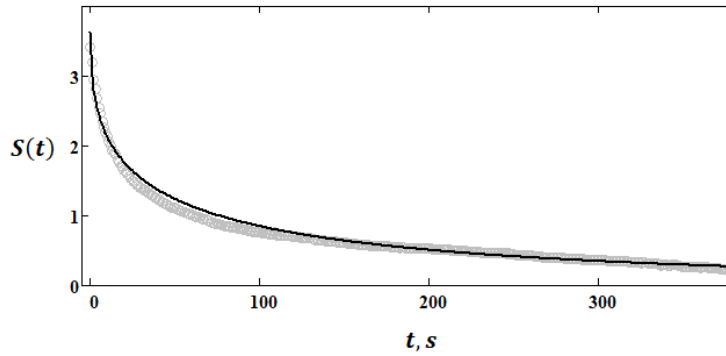


Figure 1 - Typical relaxation curve of the response of a gas sensor sample when restoring its original state. Experiment – thick curve of gray circles, approximation by a stretched exponential function – solid thin line

Below are illustrations of the actions that are implemented by the described algorithm (Figures 2 and 3).

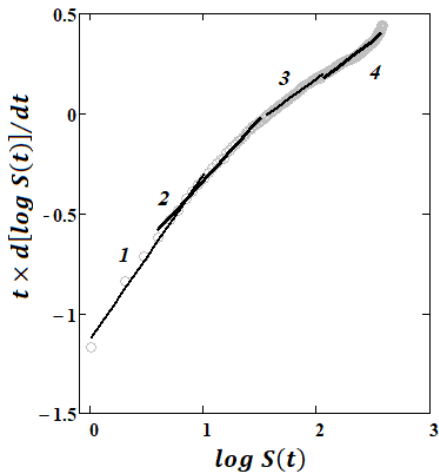


Figure 2 - Response relaxation curve Fig. 1 in coordinates $\{t \times [d \log S(t) / dt]$ and $\log S(t)\}$. Mugs are an experiment. Linear approximations at different time intervals (indicated by numbers 1, 2, 3 and 4) – solid line

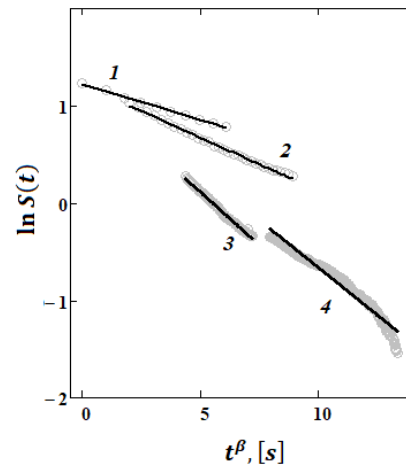


Figure 3 - Response relaxation curve Fig. 1 for different time intervals in coordinates $\{\ln S(t) \text{ и } t^\beta\}$.

The remaining designations correspond to those adopted in Fig.2.

As can be seen from Fig. 2, the entire curve can be represented by linear dependencies in each of the 4 intervals, which allows using expression (2) to find the corresponding values of this parameter β_{kj} (k is the index of the processed kinetic dependence, j is the interval index).

The unknown parameters τ и S_0 were determined by applying formula (3) for each selected interval and the corresponding, already found, values $\beta_{k,j}$ (Fig.3).

Substituting the values $\{\beta_{k,j}\}$, $\{S_{0,k,j}\}$ и $\{\tau_{k,j}\}$ into expressions (4) made it possible to obtain optimal values of the KWW - function parameters corresponding to condition (5) for each experimental kinetic dependence. In Figure 1 shows one of these approximations for comparison. As a result, tables of optimal values of the KWW parameters of the approximating functions $\{\beta_k = \beta_{k,jm}\}$, $\{S_{0k} = S_{0,k,j}\}$ and $\{\tau_k = \tau_{k,j}\}$ were obtained. At the next stage, in accordance with the operations outlined in the third paragraph of the algorithm under consideration, the selection of analytical functions $\beta_i(x_k, a_0, a_1, a_2)$, is made, which most accurately reflect the studied trends in changes in these parameters from the influence of a given factor (temperature).

The results of processing and analysis of data from experimental studies of the kinetics of the gas sensor recovery response and its dependence on temperature are shown in Fig. 4.

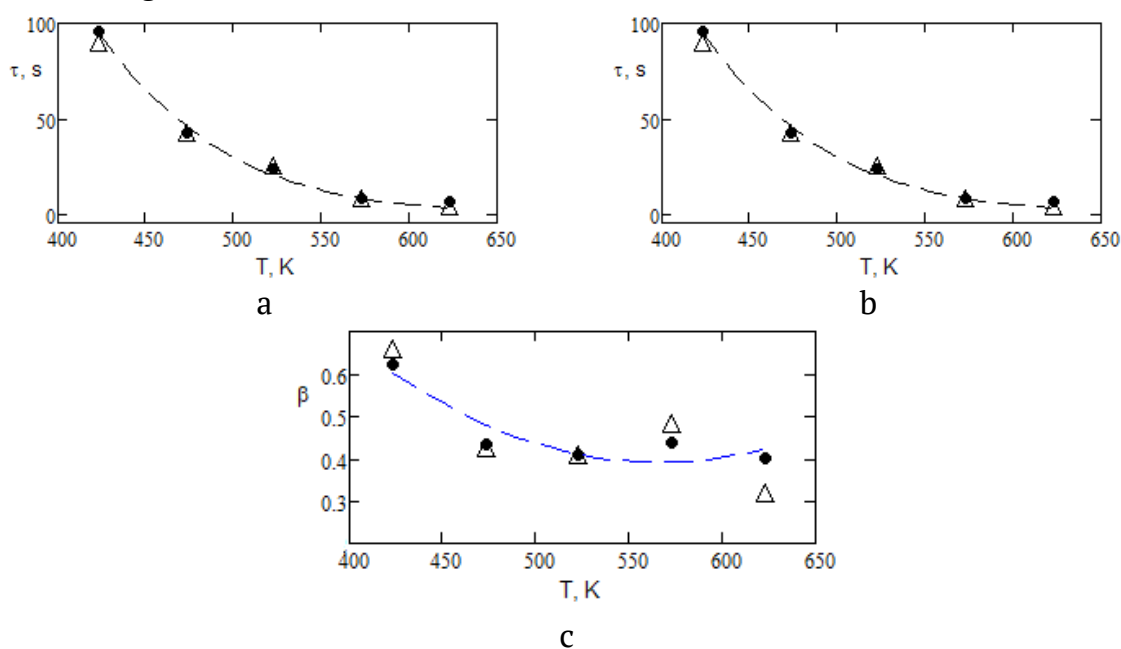


Figure 4 - The influence of temperature on the stationary (maximum) value of the response S_0 (a) and the parameters that determine the relaxation process: characteristic time τ (b) and the elongation index of the duration of this process β (c) of a sample of zinc oxide ceramics with the addition of silver oxide (1,5 wt.%) after exposure to methane (relative concentration in air 0,005%). Circles – values obtained based on the proposed data processing, triangles – data [12], dotted line – approximation results

As can be seen, the given values of $\{\beta_k\}$, $\{S0_k\}$, $\{\tau_k\}$ and their dependences on temperature are in satisfactory agreement with data obtained by other methods [12, 23], as well as existing concepts [1].

Conclusions. An algorithm for processing the experimental kinetic dependence of the response of gas sensors is proposed based on a model of a stretched exponential function with intelligent components that allow you to implement the choice:

- the most informative time interval of the processed kinetic dependencies for a more accurate assessment of all model parameters;
- optimal analytical expressions for representing trends in the influence on the parameters of the specified dependence of one or another external factor characterizing the measurement conditions.

The proposed algorithm seems promising for the implementation of automation of data processing when constructing and using information-measuring systems for studying gas-sensitive sensor materials and monitoring the parameters of gaseous media based on them.

REFERENCES

1. Tonkoshkur, A. S., Lyashkov, A. Y., & Povzlo, E. L. (2018). Kinetics of Response of ZnO-Ag Ceramics for Resistive Gas Sensor to the Impact of Methane, and its Analysis Using a Stretched Exponential Function. *Sensors and Actuators B: Chemical*. Vol. 255, Part 2. February, P. 1680-1686. <https://doi.org/10.1016/j.snb.2017.08.171>
2. Acharyya, S., Nag, S., Kimbahune, S., Ghose, A., Pal, A., & Guha, P. K. (2021). Selective discrimination of VOCs applying gas sensing kinetic analysis over a metal oxide-based chemiresistive gas sensor. *ACS sensors*, 6(6), 2218-2224.
3. Saggu, I. S., Singh, S., Chen, K., Xuan, Z., Swihart, M. T., & Sharma, S. (2023). Ultrasensitive Room-Temperature NO₂ Detection Using SnS₂/MWCNT Composites and Accelerated Recovery Kinetics by UV Activation. *ACS sensors*, 8(1), 243-253
4. A.S. Tonkoshkur, A.S. Lozovskyi Application for calculating the parameters of a gas sensor from the experimental kinetic dependence of response. *System technologies*, 2021, 2(133): 26-32. DOI 10.34185/1562-9945-2-133-2021-04
5. A.S. Tonkoshkur, A.S. Lozovskyi Software for processing and analysis of experimental data in researching of gas sensors. *System technologies*, 2022, 1(138): 175-184. DOI 10.34185/1562-9945-1-138-2022-17
6. Грачева Н.Н, Руденко Н.Б., Литвинов В.Н. Специализированное программное обеспечение для научных исследований [Электронный ресурс]: учебное посо-

бие– Электрон. дан. – зерноград: Азово-Черноморский инженерный институт ФГБОУ ВО ДГАУ, 2018. – 127 с.

7. Лазурик В. Т., Починок А. В. Модель компьютерной обработки и анализа экспериментальных данных при исследовании плазменного источника ультрафиолета. Вісник Харківського національного університету Серія «Математичне моделювання. Інформаційні технології. Автоматизовані системи управління» 2008. № 833. с.149-162.

8. Пыхалов А. А., Лам З. В., Белозерцева О. П. Математическое моделирование для компьютерной обработки сканирования твердых деформируемых тел при построении и анализе их конечно-элементных моделей //Вестник Иркутского государственного технического университета. – 2018. – Т. 22. – №. 3 (134). С. 93-111

9. Шмелев О. Я., Королев В. Ф. О компьютерной обработке результатов измерений //Вестник компьютерных и информационных технологий. – 2009. – №. 9. – С. 50-53.

10. Simdyankin S I. & Mousseau N. Relationship between dynamical heterogeneities and stretched exponential relaxation // Physical Review E. - 2003. - 68 (4). - P.104-110.

11. Trzmiel J., Weron K., Janczura J. & Placzek-Popko E. Properties of the relaxation time distribution underlying the Kohlrausch-Williams-Watts photoionization of the DX centers in CdI-xMnxTe mixed crystals // Journal of Physics Condensed Matter. - 2009. 21(34). - P.345801.

12. A.S. Tonkoshkur, A.S. Lozovskyi Algorithm for processing gas sensor's response kinetics data using extended exponential function without numerical differentiation. System technologies, 2023, 1 (144): 24-34. DOI 10.34185/1562-9945-1-144-2023-04

13. Selezneva M. S., Neusypin K. A. Development of a measurement complex with intelligent component //Measurement Techniques. – 2016. – Т. 59. – С. 916-922

14. Pawłowski, M., Kamiński, P., Kozłowski, R., Jankowski, S., & Wierzbowski, M. (2005). Intelligent measuring system for characterisation of defect centres in semi-insulating materials by photoinduced transient spectroscopy. Metrology and Measurement Systems, 12(2), 207-228.

15. Selivanova, Z. M., Kurenkov, D. S., Trapeznikova, O. V., & Nagornova, I. V. (2020, May). Intelligent information-measuring system for operational control of thermophysical properties of heat insulating materials. In Journal of Physics: Conference Series (Vol. 1546, No. 1, p. 012029). IOP Publishing.

16. Shen, K., Selezneva, M. S., Neusypin, K. A., & Proletarsky, A. V. (2017). Novel variable structure measurement system with intelligent components for flight vehicles. *Metrology and measurement systems*, 347-356.
17. Yunpeng, W., Ruixin, Y., Shaojun, N., & Zonglin, J. (2020). Deep-learning-based intelligent force measurement system using in a shock tunnel. *力学学报*, 52(5), 1304-1313
18. Orlov S. P., Vasilchenko A. N. Intelligent measuring system for testing and failure analysis of electronic devices //2016 XIX IEEE International Conference on Soft Computing and Measurements (SCM). – IEEE, 2016. – С. 401-403.
19. Тонкошкур О.С., Повзло Є.Л. Алгоритм обробки даних кінетики відгуку резистивного газового сенсору на основі моделі розтягнутої експоненціальної функції. *Системні технології. Регіональний міжвузівський збірник наукових праць*. – Вип. 1'(108) – Дніпропетровськ, 2017. – С. 129-134
20. Методи та системи штучного інтелекту: Навчальний посібник для студентів напряму підготовки 6.050101«Комп'ютерні науки» А.С. Савченко, О. О. Синельников. – К. : НАУ, 2017. – 190 с.
21. Булкин В. И., Шаронова Н. В. Математические модели знаний и их реализация с помощью алгебропредикатных структур //Булкин ВИ, Шаронова НВ–Национальный технический университет «ХПИ», Макеевский экономикогуманитарный институт. Изд.: Дмитренко ЛР, Донецк. – 2010. – 304. с.
22. Шуп Е. Т. Решение инженерных задач на ЭВМ. – Мир, 1982.- 230 с.
23. Lozovskyi, A., Lyashkov, A., Gomilko, I., & Tonkoshkur, A. (2023). Implementation of computer processing of relaxation processes investigation data using extended exponential function. *Informatyka, Automatyka, Pomiaru w Gospodarce i Ochronie Środowiska*, 13(3), 51-55.

Received 07.02.2024.

Accepted 15.02.2024.

Алгоритм комп'ютерної обробки кінетичних залежностей відгуку газового сенсора з інтелектуальними компонентами

Метою роботи є розробка алгоритму з використанням інтелектуальними компонентами, що дозволить забезпечувати обробку експериментальних даних кінетики відгуку резистивних газових сенсорів на основі алгоритму моделі розтягнутої експоненційної функції Кольрауша-Вільямса-Уоттса, без втручання оператора.

У даній статті розглядаються особливості алгоритму для розрахунку параметрів необхідних для обробки експериментальних даних для вирішення задач автоматизації досліджень матеріалів для газочутливих сенсорів.

У статті описано проблеми реалізації повної автоматизації інформаційно-вимірювальної системи для дослідження основних характеристик газочутливих сенсорів, а саме вибору найбільш інформативного інтервалу часу та оптимальних аналітичних виразів уявлення тенденцій впливу параметрів зазначеної залежності того чи іншого зовнішнього чинника, що характеризують умови вимірювання. Наведено алгоритм обробки експериментальної кінетичної залежності відгуку газових сенсорів на основі моделі розтягнутої експоненціальної функції з інтелектуальними складовими, які дозволяють вибрати найбільш інформативний інтервал часу з оброблених кінетичних залежностей.

Використання запропонованого алгоритму узгоджується з даними, отриманими іншими методами, а також існуючими концепціями.

Алгоритм видається перспективним для реалізації автоматизації обробки даних при побудові та застосуванні інформаційно-вимірювальних систем для дослідження газочутливих сенсорних матеріалів.

Tonkoshkur Oleksandr Serhiiovysh - professor of department of ECM, Oles Honchar Dnipro National University.

Lozovskyi Andrii Serhiiovysh - assistant of department of ECM, Oles Honchar Dnipro National University.

Тонкошкур Олександр Сергійович - професор кафедри ЕОМ, Дніпровський національний університет імені Олеся Гончара.

Лозовський Андрій Сергійович - аспірант кафедри ЕОМ, Дніпровський національний університет імені Олеся Гончара.