Tonkie Khimicheskie Tekhnologii = Fine Chemical Technologies.
2025;20(6):531–539 ISSN 2686-7575 (Online)

Theoretical basis of chemical technology
Теоретические основы химической технологии

UDC 541.124/128
https://doi.org/10.32362/2410-6593-2025-20-6-531-539
EDN AQQLQV

RESEARCH ARTICLE

Solution of the inverse problem for chemical reactions with chaotic dynamics

Boris V. Alekseev, Vladislav Kh. Fedotov✉, Nikolay I. Kol'tsov
I.N. Ulyanov Chuvash State University, Cheboksary, Chuvash Republic, 428015 Russia
✉ *Corresponding author, e-mail: fvh@inbox.ru*

Abstract

Objectives. To develop and test a method for solving the inverse problem of chemical kinetics for estimating the frequencies of elementary stages of complex chemical reactions occurring in a chaotic regime.

Methods. The method is based on the representation of nonstationary experimental data on reagent concentrations and the rates of their change in the form of a matrix of a particular structure.

Results. The effectiveness of the method is demonstrated by examples of reactions proceeding according to stage schemes similar to the Willamowski–Rossler mechanism, characterized by undamped aperiodic oscillations.

Conclusions. The method allows the frequencies of stages for reactions proceeding according to mechanisms with non-monotonic dynamics of any complexity to be determined with high accuracy.

Keywords

inverse problem of chemical kinetics, chaotic dynamics, nonstationary experimental data, reagent concentrations and rates of their change

Submitted: 05.03.2025
Revised: 05.05.2025
Accepted: 07.11.2025

For citation

Alekseev B.V., Fedotov V.Kh., Kol'tsov N.I. Solution of the inverse problem for chemical reactions with chaotic dynamics. *Tonk. Khim. Tekhnol. = Fine Chem. Technol*. 2025;20(6):531–539. https://doi.org/10.32362/2410-6593-2025-20-6-531-539

НАУЧНАЯ СТАТЬЯ

Решение обратной задачи для химических реакций с хаотической динамикой

Б.В. Алексеев, В.Х. Федотов✉, Н.И. Кольцов

Чувашский государственный университет им. И.Н. Ульянова, Чебоксары, Чувашская Республика, 428015 Россия

✉ *Автор для переписки, e-mail: fvh@inbox.ru*

Аннотация

Цели. Разработка и апробация метода решения обратной задачи химической кинетики по оценке частот элементарных стадий сложных химических реакций, протекающих в хаотическом режиме.

Методы. Метод основан на представлении нестационарных экспериментальных данных о концентрациях реагентов и скоростях их изменения в виде матрицы специальной структуры.

Результаты. Эффективность метода показана на примерах реакций, протекающих по стадийным схемам, аналогичным механизму Вилламовски–Росслера, и характеризующихся незатухающими апериодическими колебаниями.

Выводы. Метод позволяет с высокой точностью определить частоты стадий для реакций, протекающих по механизмам с немонотонной динамикой любой сложности.

Ключевые слова

обратная задача химической кинетики, хаотическая динамика,
нестационарные экспериментальные данные,
концентрации реагентов и скорости их изменения

Поступила: 05.03.2025
Доработана: 05.05.2025
Принята в печать: 07.11.2025

Для цитирования

Алексеев Б.В., Федотов В.Х., Кольцов Н.И. Решение обратной задачи для химических реакций с хаотической динамикой. *Тонкие химические технологии*. 2025;20(6):531–539. https://doi.org/10.32362/2410-6593-2025-20-6-531-539

INTRODUCTION

Currently, there exist a number of methods for solving the inverse problem (IP) of chemical kinetics based on nonstationary data for chemical reactions proceeding in a monotonic mode [1–3]. However, methods for solving the IP for chemical reactions with non-monotonic behavior, such as critical phenomena in particular, have not been studied in practice [4, 5]. It is also known that the IP is incorrect, and its solution is usually ambiguous [6]. Possible approaches to overcoming these difficulties and improving the accuracy of the IP solution were presented in [7–11]. The study [12] considered an IP solution for the Gray–Scott self-oscillating reaction [13] based on experimental amplitude–frequency characteristics. The authors in [14] developed an alternative method for solving the IP for the same reaction and demonstrated that the use of nonstationary values of reagent concentrations and their rates of change allows the uniqueness and accuracy of the solution to be increased.

The earliest examples of chemical reactions whose dynamic models describe chaotic oscillations within the framework of the law of active masses (LAM) were demonstrated by Rossler [15]. Among them, the Willamowski–Rossler mechanism was the simplest [16–18]. In these works, the kinetic parameters of stage diagrams were determined numerically based on the conditions of instability of solutions of ordinary differential equations (ODEs) describing nonstationary models of the corresponding reactions and known criteria of chaos in dynamic systems (Lyapunov exponents, etc.) [19–20].

In this article, we present a method for solving the IP for chemical reactions with unpredictable chaotic dynamics based on data on reagent concentrations and their rates of change.

EXPERIMENTAL

The mechanism of a complex chemical reaction is described by a set of elementary stages

$$\sum b_{+ik}\mathrm{A}_k + \sum a_{+ij}\mathrm{X}_j \leftrightarrow \sum a_{-ij}\mathrm{X}_j + \sum b_{-ik}\mathrm{A}_k, \quad (1)$$

$i = 1, \ldots, s, j = 1, \ldots, n,$

wherein $b_{\pm ik}$, $a_{\pm ij}$ are the stoichiometric coefficients of reagents A_k and X_j, respectively, in the forward

and reverse directions of stage *i*. Let A_k be reagents whose concentrations remain virtually unchanged during the reaction (referred to as non-key, slow reagents in terms of the Bodenstein–Semenov quasi-stationarity principle [21]); X_j are the key reagents whose concentrations change during the reaction (essential reagents in terms of A.M. Zhabotinsky [22]). The dynamics of such a reaction in an isothermal zero-gradient reactor, according to LAM, is described by the ODE system [1]:

$$x'_j = \sum (a_{-ij} - a_{+ij})(w_i \Pi_j x_j^{a+ij} - w_{-i} \Pi_j x_j^{a-ij}),$$
$$j = 1, \ldots, n, \quad (2)$$

wherein $x_j = x_j(t)$ are the concentrations of key reagents x_j (dimensionless, dim.); t is time (s); $x_j(t_0) = x_j^0$ are the initial conditions (i.c.); t_0 is the initial moment of time (s); $w_i = k_i \Pi_k A_k^{b+ik}$, $w_{-i} = k_{-i} \Pi_k A_k^{b-ik}$ are the frequencies of forward and reverse stages, including concentration multipliers of non-key reagents (s^{-1}); k_i, k_{-i} are the constants of stage velocities in the forward and reverse directions (s^{-1}).

In the presence of experimental data on concentrations and rates of change of reagent concentrations, system (2) is a linear system of algebraic equations with respect to stage frequencies, which can be written as

$$v_j = \sum (a_{-ij} - a_{+ij})(w_i r_{ij} - w_{-i} r_{-ij}), j = 1, \ldots, n, \quad (3)$$

wherein v_j are the rates of change in the concentrations of key reagents; r_{ij}, r_{-ij} are the monomials of the stage rates, i.e., the stage rates at single values of the stage frequencies. Dividing the right-hand side of system (3) into monomials and frequencies is convenient, since the numerical values of the monomials are known from the experiment at each time point (they are equal to the product of the concentrations of key reagents), and the values of the frequencies of the stages are the desired parameters of the IP.

System (3) typically includes identical stage velocity monomials with different stage frequency values. Let us combine such monomials (bring similar ones together) and write down system (3) modified in this way in a concise (matrix) form

$$\mathbf{v} = \mathbf{R}\mathbf{w}, \quad (3^*)$$

wherein $\mathbf{R}$ is the matrix of various monomials of velocities (after reduction of similar ones), $\mathbf{w}$ is a vector of stage frequencies.

The best solution to such a system is provided by methods for minimizing the error function $f(\mathbf{w})$ (penalty function), e.g. , in the form of a sum of squared deviations

$$f(\mathbf{w}) = (\mathbf{R}\mathbf{w} - \mathbf{v})^{\mathrm{T}} (\mathbf{R}\mathbf{w} - \mathbf{v}), \quad (4)$$

wherein T is the transpose sign. This solution can be written using the pseudo-inverse matrix $\mathbf{R}^+$ [23]:

$$\mathbf{w} = \mathbf{R}^+ \mathbf{v}. \quad (5)$$

In a special case when the original matrix $\mathbf{R}$ is square and non-degenerate, the pseudo-inverse matrix coincides with the inverse $\mathbf{R}^+ = \mathbf{R}^{-1}$. In the general case, when the number of experimental points is not equal to the number of desired stage frequencies, the matrix $\mathbf{R}$ has an incomplete rank. Then, if the product of the matrices $\mathbf{R}^{\mathrm{T}}\mathbf{R}$ is not degenerate, then

$$\mathbf{R}^+ = (\mathbf{R}^{\mathrm{T}}\mathbf{R})^{-1}\mathbf{R}^{\mathrm{T}}, \quad (6)$$

wherein $\mathbf{R}^{\mathrm{T}}$ is the transposed matrix. If the product $\mathbf{R}^{\mathrm{T}}\mathbf{R}$ has an incomplete rank, then

$$\mathbf{R}^+ = \lim_{\delta \to 0} (\mathbf{R}^{\mathrm{T}}\mathbf{R} + \delta\mathbf{E})^{-1}\mathbf{R}^{\mathrm{T}}, \quad (7)$$

wherein $\mathbf{E}$ is the identity matrix. Calculations performed in computer algebra systems [3, 24] have shown the insufficiency of formula (6) to determine the frequencies of the stages.

For comparison, we also use the penalty function, i.e., the maximum of deviation modules.

$$f(\mathbf{w}) = \max(abs(\mathbf{R}\mathbf{w} - \mathbf{v})). \quad (8)$$

Function (8) is a composition of functions **max** and *abs*, having kinks, and its analysis is more complicated than the analysis of function (4). The minimum of function (8) can be found by dividing the entire space of possible values of the vector $\mathbf{w}$ into regions of smoothness (8), finding the minimum in each of these regions and then selecting the global minimum from these local minima. Obviously, the minimum points of functions (4) and (8) are different, and these minima correspond to different values of the vector $\mathbf{w}$.

RESULTS AND DISCUSSION

Let us apply the method described above to reactions proceeding according to stepwise schemes similar to the Willamowski–Rossler mechanism, characterized by continuous aperiodic (chaotic) oscillations [15–18, 25, 26].

Example 1. Let us consider the homogeneous reaction A + 2B → C + D proceeding according to the scheme [25]:

$$1)\ A + X \leftrightarrow 2X,\ 2)\ B + X + Y \rightarrow 2Y + A,$$
$$3)\ Z + Y \rightarrow D,\ 4)\ A + B \rightarrow Z + C. \quad (1.1)$$

wherein A, B, C, and D are the non-key reagents (can be any); X, Y, and Z are the key reagents. According to this scheme, the reaction $CO + 2NO \rightarrow N_2O + CO_2$ can occur:

$$1)\ CO + CO^* \leftrightarrow 2CO^*,$$
$$2)\ NO + CO^* + NO^* \rightarrow 2NO^* + CO, \quad (1.2)$$
$$3)\ N^* + NO^* \rightarrow N_2O,\ 4)\ CO + NO \rightarrow N^* + CO_2.$$

An unsteady kinetic model of reactions proceeding according to schemes (1.1) and (1.2), under the assumption of quasi-stationarity for non-key reagents, is described by

$$\begin{aligned} x' &= w_1 x - w_{-1} x^2 - w_2 xy, \\ y' &= w_2 xy - w_3 yz, \\ z' &= -w_3 yz + w_4, \end{aligned} \qquad (1.3)$$

wherein w_i, w_{-i} are the frequencies of steps in the forward and reverse directions, including the concentrations of non-key reagents; x, y, and z are the concentrations of key reagents X, Y, and Z. It was shown in [25] that system (1.3) exhibits chaotic oscillations at certain values of the frequencies of stages and current levels (Fig. 1).

The concentrations of key reagents and their rates of change, selected for calculations at certain time points from dependencies $x(t)$, $y(t)$, $z(t)$ (Fig. 1), are shown in Table 1.

Equations (1.3) contain five different monomials of velocities 1, x, x^2, xy, yz. They form a matrix **R** of size $5 \times 3n$, made up of triples of rows $[0, x, -x^2, -xy, 0]$, $[0, 0, 0, xy, -yz]$, and $[1, 0, 0, 0, -yz]$ for reagents X, Y, and Z, respectively, calculated for each experiment. The results of the IP solution for two variants of the penalty function (4) and (8) are given in Table 2.

It can be seen from Table 2 that the errors in determining the frequency of stages by the method described above are small for both methods of selecting the penalty function.

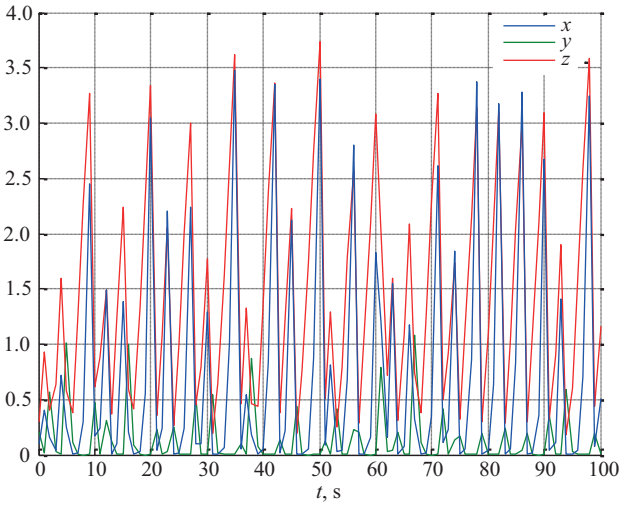

Fig. 1. Dependencies $x(t)$, $y(t)$, $z(t)$ in the reaction A + 2B → C + D described by model (1.3) at $w_1 = 3$, $w_{-1} = 0.75$, $w_2 = 18$, $w_3 = 10$, $w_4 = 1$ s^{-1}, and $x_0 = 0.1$, $y_0 = 0.2$, $z_0 = 0.3$

Table 1. Concentrations of reagents and rates of their change* in the reaction A + 2B → C + D, proceeding according to scheme (1.1) at $w_1 = 3$, $w_{-1} = 0.75$, $w_2 = 18$, $w_3 = 10$, $w_4 = 1$, s^{-1}

t, s	0	5	10	15	20	25
x, a.u.	0.1000	0.2480	0.1663	1.3908	3.0491	0.0127
y, a.u.	0.2000	1.0100	0.4738	0.0000	0.0000	0.0009
z, a.u.	0.3000	0.5827	0.6112	2.2368	3.3339	1.0031
x', s^{-1}	−0.0675	−3.8114	−0.9403	2.7217	2.1732	0.0376
y', s^{-1}	−0.2400	−1.3758	−1.4775	0.0000	0.0006	−0.0088
z', s^{-1}	0.4000	−4.8852	−1.8960	1.0000	0.9991	0.9910

* The rates of change of reagent concentrations x', y', z' are calculated using equations (1.3).

Table 2. Accuracy of the IP solution for reaction (1.1) depending on the penalty function

Penalty function	Stage frequencies	w_1, s^{-1}	w_2, s^{-1}	w_3, s^{-1}	w_4, s^{-1}	w_{-1}, s^{-1}
	The exact value	3.00	18.00	10.00	1.00	0.75
(4)	Estimated value	3.0008	18.0031	9.9998	0.9998	0.7504
	Error rate, %	0.0267	0.0172	0.0020	0.0200	0.0533
(8)	Estimated value	3.0004	18.0029	9.9989	0.9994	0.7503
	Error rate, %	0.0133	0.0161	0.0110	0.0600	0.0400

Example 2. Let us consider the heterogeneous catalytic reaction of $2NO + CO \rightarrow N_2O + CO_2$, occurring on platinum metals according to the step scheme [26]:

$$\begin{aligned} &1)\ CO + Q + QCO \leftrightarrow 2QCO,\\ &2)\ NO + QCO + QN \rightarrow 2QN + CO_2,\\ &3)\ QNO + QN \rightarrow 2Q + N_2O,\ 4)\ NO + Q \rightarrow QNO, \end{aligned} \qquad (2.1)$$

wherein the key reagents are QCO, QN, and QNO are the catalyst surface centers occupied by carbon monoxide and nitrogen, and Q are free catalyst centers. Briefly, without the non-key reagents NO, CO, N_2O, and CO_2, scheme (2.1) takes the form

$$1)\ Q + X \leftrightarrow 2X,\ 2)\ X + Y \rightarrow 2Y,\quad 3)\ Z + Y \rightarrow 2Q,\ 4)\ Q \rightarrow Z, \qquad (2.2)$$

for which the kinetic model (2) can be written as:

$$\begin{aligned} x' &= w_1xq - w_{-1}x^2 - w_2xy,\\ y' &= w_2xy - w_3yz,\\ z' &= -w_3yz + w_4q, \end{aligned} \qquad (2.3)$$

wherein x, y, z, and q are the dimensionless concentrations of key substances QCO = X, QN = Y, QNO = Z and free centers Q on the surface of the catalyst, with $x + y + z + q = 1$ (the law of conservation of the catalyst). It should be noted that the concentrations of key substances and free centers on the surface of the catalyst cannot be measured even by modern physicochemical research methods. It was shown in [26] that the ODE system (2.3) describes chaotic oscillations at certain values of the frequencies of stages and initial conditions (Fig. 2).

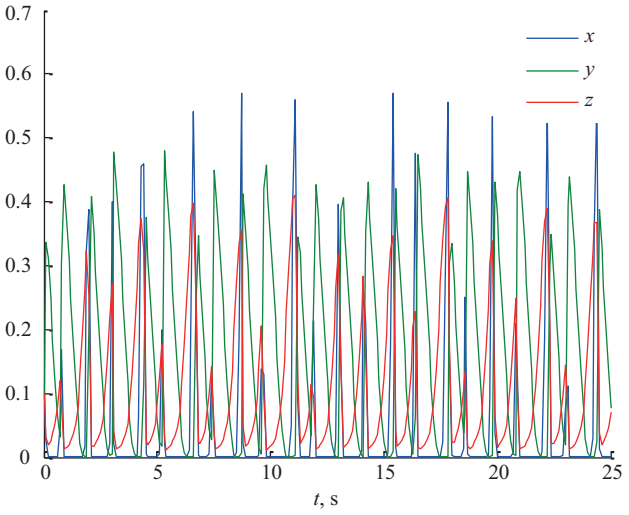

Fig. 2. Dependencies $x(t)$, $y(t)$, $z(t)$ in reaction of interaction of nitrogen and carbon monoxides described by model (2.3) at $w_1 = 50$, $w_2 = 200$, $w_3 = 100$, $w_4 = w_{-1} = 1\ s^{-1}$, $x_0 = y_0 = z_0 = 0.1$

The values of reagent concentrations and their rates of change, selected for calculations at certain time points from dependencies $x(t)$, $y(t)$, $z(t)$ (Fig. 2), are shown in Table 3.

Equations (2.3) contain five different monomials of velocities xq, xy, yz, q, x^2. They form a matrix **R** of size $5 \times 3n$, composed of triples of rows $[xq, -xy, 0, 0, -x^2]$, $[0, xy, -yz, 0, 0]$, and $[0, 0, -yz, q, 0]$ for reagents X, Y, and Z, respectively, calculated for each experiment. The IP solution for penalty functions (4) and (8) are given in Table 4.

Table 3. Concentrations of reagents and rates of their change in the reaction of interaction of nitrogen and carbon monoxides, proceeding according to mechanism (2.1) at $w_1 = 50$, $w_2 = 200$, $w_3 = 100$, $w_4 = w_{-1} = 1\ s^{-1}$

t, s	0	1	2	3	4	5
x, a.u.	0.1000	0.0000	0.3869	0.4011	0.0000	0.0002
y, a.u.	0.1000	0.3701	0.1965	0.0047	0.0044	0.0640
z, a.u.	0.1000	0.0156	0.2543	0.2714	0.1935	0.0787
x', s^{-1}	1.4900	−0.0001	−12.2097	5.9310	0.0018	0.0057
y', s^{-1}	1.0000	−0.5788	10.2050	0.2518	−0.0853	−0.5017
z', s^{-1}	−0.3000	0.0353	−4.8335	0.1940	0.7167	0.3530

Table 4. Dependence of the IP solution accuracy on the choice of the penalty function for the reaction of interaction of nitrogen and carbon monoxides, proceeding according to scheme (2.1)

Penalty function	Stage frequencies	w_1, s^{-1}	w_2, s^{-1}	w_3, s^{-1}	w_4, s^{-1}	w_{-1}, s^{-1}
	The exact value	50.00	200	100	1	1
(4)	Estimated value	49.9728	199.9172	99.9609	1.0020	0.9986
	Error rate, %	0.0544	0.0414	0.0391	0.2000	0.1400
(8)	Estimated value	49.9533	199.9042	99.9130	1.0085	0.9953
	Error rate, %	0.0934	0.0479	0.0870	0.8500	0.4700

It can be seen from Table 4 that the errors in determining the stage frequencies for both variants of penalty functions (4) and (8) are quite small. The found values of the stage frequencies for different penalty functions are almost the same.

CONCLUSIONS

A method for solving the inverse kinetic problem for reactions proceeding by mechanisms with chaotic dynamics is proposed. This method is based on the use of experimentally measured values of reagent concentrations and their rates of change. The proposed approach differs from the previously known methods in the isolation of different stage velocity monomials and the method of forming the experimental data matrix. According to the conducted analysis, the described method makes it possible to accurately determine the frequencies of stages for reactions proceeding through mechanisms with dynamics of any complexity (monotonous, non-monotonous, periodic, and chaotic).

Authors' contributions

B.V. Alekseev—development of methods and algorithms for solving inverse problems, software development, planning and conducting computational experiments, analysis of results.

V.Kh. Fedotov—problem statement, planning and conducting computational experiments, analysis of results, writing the text of the article.

N.I. Kol'tsov—statement of the research goal and objectives, analysis of the obtained results, writing the text of the article.

All authors approved the final version of the article.

The authors declare no conflict of interest.

REFERENCES

1. Ismagilova A.S., Spivak S.I. *Obratnye zadachi khimicheskoi kinetiki* (*Inverse Problems of Chemical Kinetics*). Saarbrucken: Lap Lambert Academic Publ.; 2013, 125 p. (In Russ.). ISBN 978-36593118474. https://www.elibrary.ru/glykiv
2. Yagola A.G., Yanfei V., Stepanova I.EH., Titarenko V.N. *Obratnye zadachi i metody ikh resheniya. Prilozheniya k geofizike* (*Inverse Problems and Methods of their Solution. Applications to Geophysics*). Moscow: Laboratoriya znanii; 2021, 217 p. (In Russ.). ISBN 978-5-93208-555-4
3. Leonov A.S. *Reshenie nekorrektno postavlennykh obratnykh zadach: ocherk teorii, prakticheskie metody i demonstratsii v MATLAB* (*Solution of ill-Posed Inverse Problems: Outline of theory, Practical Methods and Demonstrations in MATLAB*). Moscow: Librokom; 2024, 368 p. (In Russ.). ISBN 978-5-9710-9965-9
4. Pisarenko E.V., Pisarenko V.N. Analysis and simulation of the nonlinear kinetics of reacting chemical systems. *Theor. Found. Chem. Eng*. 2013;47(2):128–135. https://doi.org/10.1134/S004057951302005X
[Original Russian Text: Pisarenko E.V., Pisarenko V.N. Analysis and simulation of the nonlinear kinetics of reacting chemical systems. *Teoreticheskie Osnovy Khimicheskoi Tekhnologii*. 2013;47(2): 173–181 (in Russ.). https://doi.org/10.7868/S0040357113020061]
5. Shatalov M.Y., Fedotov S.I., Shatalov Y.M. New methods of determination of kinetic parameters of the theoretical models from experimental data. *Theor. Found. Chem. Eng*. 2013;47(3): 207–216. https://doi.org/10.1134/S0040579513020097
[Original Russian Text: Shatalov M.Yu., Fedotov S.I., Shatalov Yu.M. New methods of determination of kinetic parameters of the theoretical models from experimental data. *Teoreticheskie Osnovy Khimicheskoi Tekhnologii*. 2013;47(3):260–270 (in Russ.). https://doi.org/10.7868/S0040357113020103]
6. Gorsky V.G. *A prior parameter identifiability analysis of fixed structure models.* In: Letzky E.K. (Ed.). *Design of Experiments and Data Analysis: New Trends and Results*. Moscow: Antal; 1993. P. 92–131.

СПИСОК ЛИТЕРАТУРЫ

1. Исмагилова А.С., Спивак С.И. *Обратные задачи химической кинетики*. Saarbrucken: Lap Lambert Academic Publ.; 2013, 125 с. ISBN 978-36593118474. https://www.elibrary.ru/glykiv
2. Ягола А.Г., Янфей В., Степанова И.Э., Титаренко В.Н. *Обратные задачи и методы их решения. Приложения к геофизике*. М.: Лаборатория знаний; 2021, 217 с. ISBN 978-5-93208-555-4
3. Леонов А.С. *Решение некорректно поставленных обратных задач: очерк теории, практические методы и демонстрации в МАТЛАБ*. М.: Либроком; 2024, 368 с. ISBN 978-5-9710-9965-9
4. Писаренко Е.В., Писаренко В.Н. Анализ и моделирование нелинейной кинетики химических реагирующих систем. *Теор. основы хим. технологии*. 2013;47(2):173–181. https://doi.org/10.7868/S0040357113020061
5. Шаталов М.Ю., Федотов С.И., Шаталов Ю.М. Новый метод определения кинетических параметров теоретических моделей на основе экспериментальных данных. *Теор. основы хим. технологии*. 2013;47(3):260–270. https://doi.org/10.7868/S0040357113020103
6. Gorsky V.G. *A prior parameter identifiability analysis of fixed structure models.* In: Letzky E.K. (Ed.). *Design of Experiments and Data Analysis: New Trends and Results*. Moscow: Antal; 1993. P. 92–131.
7. Федотов В.Х., Кольцов Н.И. Разработка метода решения обратной задачи химической кинетики для каталитических реакций с участием основных веществ в каждой стадии. *Хим. физика*. 2016;35(10):9–15. https://doi.org/10.7868/S0207401X1610006X
8. Кольцов Н.И. Метод решения обратной задачи химической кинетики многостадийных реакций. *Кинетика и катализ*. 2020;61(6):783–788. https://doi.org/10.31857/S0453881120040127
9. Кольцов Н.И. Метод определения констант скоростей стадий химических реакций в закрытом безградиентном реакторе. *Журн. прикладной химии*. 2020;93(10):1474–1481. https://doi.org/10.31857/S0044461820100096

7. Fedotov V.Kh., Kol'tsov N.I. Method of solving the inverse problem of chemical kinetics for catalytic reactions in which each step involves main reactants. *Rus. J. Phys. Chem. B*. 2016;10(5): 753–759. https://doi.org/10.1134/S1990793116050195
[Original Russian Text: Fedotov V.Kh., Kol'tsov N.I. Method of solving the inverse problem of chemical kinetics for catalytic reactions in which each step involves main reactants. *Khimicheskaya Fizika*. 2016;35(10):9–15 (in Russ.). https://doi.org/10.7868/S0207401X1610006X]
8. Kol'tsov N.I. Method for Solving the Inverse Problem of the Chemical Kinetics of Multistage Reactions. *Kinet. Catal*. 2020;61(6):833–838.https://doi.org/10.1134/S0023158420040096
[Original Russian Text: Kol'tsov N.I. Method for Solving the Inverse Problem of the Chemical Kinetics of Multistage Reactions. *Kinetika i Kataliz*. 2020;61(6):783–788 (in Russ.). https://doi.org/10.31857/S0453881120040127]
9. Kol'tsov N.I. Method for Determining the Rate Constants of Chemical Reaction Stages in an Enclosed Gradientless Reactor. *Russ. J. Applied Chem*. 2020;93(10):1544–1552. https://doi.org/10.1134/S1070427220100092
[Original Russian Text: Kol'tsov N.I. Method for Determining the Rate Constants of Chemical Reaction Stages in an Enclosed Gradientless Reactor. *Zhurnal Prikladnoi Khimii*. 2020;93(10):1474–1481 (in Russ.). https://doi.org/10.31857/S0044461820100096]
10. Kol'tsov N.I. Solving the Inverse Problem for Chemical Reactions Occurring in a Plug-Flow Reactor. *Theor. Found. Chem. Eng*. 2021;55(6):1238–1245. https://doi.org/10.1134/S0040579521050237
[Original Russian Text: Kol'tsov N.I. Solving the Inverse Problem for Chemical Reactions Occurring in a Plug-Flow Reactor. *Teoreticheskie Osnovy Khimicheskoi Tekhnologii*. 2021;55(6):772–779 (in Russ.). https://doi.org/10.31857/S0040357121050043]
11. Kol'tsov N.I., Fedotov V.Kh. *Invarianty i obratnye zadachi khimicheskoi kinetiki* (*Invariants and Inverse Problems of Chemical Kinetics*). Cheboksary: Chuvash University Publ.; 2022, 240 p. (In Russ.). ISBN 978-5-7677-3431-3
12. Katsman E.A., Sokolova I.V., Temkin O.N. Solution of reverse kinetic problem for oscillatory reactions. *Theor. Found. Chem. Eng*. 2014;48(2):175–179. https://doi.org/10.1134/S0040579514020067
[Original Russian Text: Katsman E.A., Sokolova I.V., Temkin O.N. Solution of reverse kinetic problem for oscillatory reactions. *Teoreticheskie Osnovy Khimicheskoi Tekhnologii*. 2014;48(2): 190–195 (in Russ.). https://doi.org/10.7868/S0040357114020067]
13. Gray P., Scott S.K. *Chemical Oscillations and Instabilities. Non-linear Chemical Kinetics*. Oxford: Clarendon Press; 1994, 470 p.
14. Alekseev B.V., Fedotov V.Kh., Kol'tsov N.I. Solution of the inverse problem of chemical kinetics for oscillatory reactions. *Theor. Found. Chem. Eng*. 2025. (In press).
15. Rössler O.E. Chaotic behavior in simple reaction system. *Z. Naturfosch*. 1976;A(31):259–264. https://doi.org/10.1515/zna-1976-3-408
16. Willamowski K.D., Rössler O.E. Irregular oscillations in a realistic abstract quadratic mass action system. *Z. Naturforsch*. 1980;35a:317–318. https://doi.org/10.1515/zna-1980-0308
17. Gaspard P. Rössler systems. In: *Encyclopedia of Nonlinear Science*. New York: Routledge; 2005. P. 808–811.
18. Stucki J., Urbanczik R. Entropy Production of the Willamowski-Rossler Oscillator. *Z. Naturforsch*. 2005;60a:599–607. https://doi.org/10.1515/zna-2005-8-907
19. Shuster G. *Determinirovannyi khaos: Vvedenie* (*Deterministic Chaos: An Introduction*): transl. from Engl. Moscow: Mir; 1988, 248 p. (In Russ.). ISBN 5-03-001373-3
10. Кольцов Н.И. Решение обратной задачи для химических реакций, протекающих в реакторе идеального вытеснения. *Теор. основы хим. технологии*. 2021;55(6):772–779. https://doi.org/10.31857/S0040357121050043
11. Кольцов Н.И., Федотов В.Х. *Инварианты и обратные задачи химической кинетики*. Чебоксары: Изд-во Чуваш. ун-та; 2022, 240 с. ISBN 978-5-7677-3431-3
12. Кацман Е.А., Соколова И.В., Темкин О.Н. Решение обратной кинетической задачи для колебательных реакций. *Теор. основы хим. технологии*. 2014;48(2):190–195. https://doi.org/10.7868/S0040357114020067
13. Gray P., Scott S.K. *Chemical Oscillations and Instabilities. Non-linear Chemical Kinetics*. Oxford: Clarendon Press; 1994, 470 p.
14. Алексеев Б.В., Федотов В.Х., Кольцов Н.И. Решение обратной задачи химической кинетики для колебательных реакций. *Теорет. основы хим. технологии*. 2025 (в печати).
15. Rössler O.E. Chaotic behavior in simple reaction system. *Z. Naturfosch*. 1976;A(31):259–264. https://doi.org/10.1515/zna-1976-3-408
16. Willamowski K.D., Rössler O.E. Irregular oscillations in a realistic abstract quadratic mass action system. *Z. Naturforsch*. 1980;35a:317–318. https://doi.org/10.1515/zna-1980-0308
17. Gaspard P. Rössler systems. In: *Encyclopedia of Nonlinear Science*. New York: Routledge; 2005. P. 808–811.
18. Stucki J., Urbanczik R. Entropy Production of the Willamowski-Rossler Oscillator. *Z. Naturforsch*. 2005;60a:599–607. https://doi.org/10.1515/zna-2005-8-907
19. Шустер Г. *Детерминированный хаос: Введение:* пер. с англ. М.: Мир; 1988, 248 с. ISBN 5-03-001373-3
20. Кузнецов С.П. *Динамический хаос*. М.: Физматлит; 2006, 356 с. ISBN 5-94052-100-2
21. Киперман С.Л. *Основы химической кинетики в гетерогенном катализе*. М.: Химия; 1979, 352 с.
22. Жаботинский А.М. *Концентрационные автоколебания*. М.: Наука; 1974, 179 с.
23. Выгодский М.Я. *Справочник по высшей математике*. М.: АСТ; 2019, 703 с. ISBN 978-5-17-117741-6
24. Аладьев В.З. *Системы компьютерной алгебры: Maple: Искусство программирования*. М.: Лаборатория Базовых Знаний; 2006, 792 с. ISBN 5-93208-189-9
25. Кольцов Н.И. Хаотические колебания в простейшей химической реакции. *Известия высших учебных заведений. Химия и хим. технол*. 2018;61(4-5):133–135. https://doi.org/10.6060/tcct.20186104-05.5654
26. Кольцов Н.И, Федотов В.Х. Хаотические колебания в простой гетерогенно-каталитической реакции. *Бутлеровские сообщения*. 2017;50(6):30–33. https://elibrary.ru/zefnpr

20. Kuznetsov S.P. *Dinamicheskii khaos* (*Dynamic Chaos*). Moscow: Fizmatlit; 2006, 356 p. (In Russ.). ISBN 5-94052-100-2
21. Kiperman S.L. *Osnovy khimicheskoi kinetiki v geterogennom katalize* (*Fundamentals of Chemical Kinetics in Heterogeneous Catalysis*). Moscow: Khimiya; 1979, 352 p. (In Russ.).
22. Zhabotinskii A.M. *Kontsentratsionnye avtokolebaniya* (*Concentration Self-Oscillations*). Moscow: Nauka; 1974, 179 p. (In Russ.).
23. Vygodskii M.Ya. *Spravochnik po vysshei matematike* (*Handbook of Higher Mathematics*). Moscow: AST; 2019, 703 p. (In Russ.). ISBN 978-5-17-117741-6
24. Alad'ev V.Z. *Sistemy komp'yuternoi algebry: Maple: Iskusstvo programmirovaniya* (*Computer Algebra Systems: Maple: The Art of Programming*). Moscow: Laboratoriya Bazovykh Znanii; 2006, 792 p. (In Russ.). ISBN 5-93208-189-9
25. Kol'tsov N.I. Chaotic oscillations in the simplest chemical reaction. *ChemChemTech = Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.* 2018;61(4-5):133–135 (in Russ.). https://doi.org/10.6060/tcct.20186104-05.5654
26. Kol'tsov N.I., Fedotov V.Kh. Chaotic oscillations in a simple heterogeneous catalytic reaction. *Butlerovskie soobshcheniya = Butlerov Communications*. 2017;50(6):30–33 (in Russ.). https://elibrary.ru/zefnpr

About the Authors

Boris V. Alekseev, Cand. Sci. (Phys.-Math.), Associate Professor, Department of Physical Chemistry and Macromolecular Compounds, I.N. Ulyanov Chuvash State University (15, Moskovskii pr., Cheboksary, 428015, Russia). E-mail: a402539@yandex.ru. Scopus Author ID 7005563886, ResearcherID GNO-9997-2022, RSCI SPIN-code 7478-3333, https://orcid.org/0000-0003-1971-0806

Vladislav Kh. Fedotov, Cand. Sci. (Chem.), Associate Professor, Department of Physical Chemistry and Macromolecular Compounds, I.N. Ulyanov Chuvash State University (15, Moskovskii pr., Cheboksary, 428015, Russia). E-mail: fvh@inbox.ru. Scopus Author ID 8863837600, ResearcherID B-6529-2017, RSCI SPIN-code 5111-9580, https://orcid.org/0000-0001-8395-6849

Nikolay I. Kol'tsov, Dr. Sci. (Chem.), Professor, Head of the Department of Physical Chemistry and Macromolecular Compounds, I.N. Ulyanov Chuvash State University (15, Moskovskii pr., Cheboksary, 428015, Russia). E-mail: koltsovni@mail.ru. Scopus Author ID 7003771176, ResearcherID O-1354-2017, RSCI SPIN-code 4229-2226, https://orcid.org/0000-0003-2264-1370

Об авторах

Алексеев Борис Васильевич, к.ф.-м.н., доцент кафедры физической химии и высокомолекулярных соединений, ФГБОУ ВО «Чувашский государственный университет имени И.Н. Ульянова» (428015, Россия, г. Чебоксары, Московский пр-т, д. 15). E-mail: a402539@yandex.ru. Scopus Author ID 7005563886, ResearcherID GNO-9997-2022, SPIN-код РИНЦ 7478-3333, https://orcid.org/0000-0003-1971-0806

Федотов Владислав Харитонович, к.х.н., доцент кафедры физической химии и высокомолекулярных соединений, ФГБОУ ВО «Чувашский государственный университет имени И.Н. Ульянова» (428015, Россия, г. Чебоксары, Московский пр-т, д. 15). E-mail: fvh@inbox.ru. Scopus Author ID 8863837600, ResearcherID B-6529-2017, SPIN-код РИНЦ 5111-9580, https://orcid.org/0000-0001-8395-6849

Кольцов Николай Иванович, д.х.н., профессор, заведующий кафедрой физической химии и высокомолекулярных соединений, ФГБОУ ВО «Чувашский государственный университет имени И.Н. Ульянова» (428015, Россия, г. Чебоксары, Московский пр-т, д. 15). E-mail: koltsovni@mail.ru. Scopus Author ID 7003771176, ResearcherID O-1354-2017, SPIN-код РИНЦ 4229-2226, https://orcid.org/0000-0003-2264-1370

Translated from Russian into English by N. Isaeva
Edited for English language and spelling by Dr. David Mossop