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Satbayev University

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ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ
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A METHOD FOR ACCOUNTING THE IMPACT OF ERRORS ON THE QUALITY OF ANALYTICAL INSTRUMENTS AND OPTIMAL CONTROL SYSTEMS

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Abstract. In various spheres of the economy and life of society, including in the oil and gas and mining industries, in geology, in metallurgy and in many other areas of industry, design and research work is currently being actively carried out to ensure successful innovative development in the design and implementation of new improved analytical devices and control systems. At the same time, at the stages of design, manufacture and practical application of analytical instruments and systems, for objective reasons, there are or occur errors that further affect the quality of technological complexes or control systems as a whole. In this paper, based on modeling and analysis of some topical problems, we consider a method for taking into account the influence of errors on the main parameters and characteristics of analytical instruments and optimal control systems. As one of the main problems, we consider the effect of technological errors on the electron-optical parameters of ion sources, which are built on the basis of cathode lenses with a hollow cathode and are one of the main components of various types of mass spectrometers, the resolution and sensitivity of which largely determine the capabilities in the field of analysis of the composition of various minerals, chemical elements and their mixtures. It is further shown that the method proposed by the authors of the article can be applied to solve problems of analyzing the influence of errors on the optimality indicators of control systems for technical complexes and technological processes in various industries and the economy. The results of the work can be used to analyze and evaluate the impact of various types of errors on the quality of specific instruments and process control systems.

Keywords: minerals and mixtures, analysis, mass spectrometer, process error, optimal control, method, quality

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АУЫТҚУЛАРДЫҢ АНАЛИТИКАЛЫҚ АСПАПТАР МЕН ОПТИМАЛДЫ БАСҚАРУ ЖҮЙЕЛЕРІНІҢ САПАСЫНА ӘСЕРІН ЕСКЕРУ ТӘСІЛІ

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Аннотация. Экономиканың және қоғамдық шаруалардың түрлі салаларында, оның ішінде мұнай-газ және тау-кен өндіру салаларында, геологияда, металлургияда және өнеркәсіптің басқа да көптеген салаларында қазіргі уақытта табысты инновациялық дамуды қамтамасыз ету үшін жаңа жетілдірілген аналитикалық аспаптар мен басқару жүйелерін жобалап іске қосу бағытында жобалау және зерттеу жұмыстары белсенді жүргізілуде. Бұл жағдайда объективті себептер бойынша аналитикалық аспаптар мен жүйелерді жобалау, дайындау және практикалық қолдану кезеңдерінде пайда болған ауытқулар әріде технологиялық кешендердің немесе тұтастай басқару жүйелерінің сапасына әсер етеді. Бұл жұмыста, кейбір өзекті мәселелерді модельдеу және талдау негізінде, ауытқулардың аналитикалық құрылғылар мен оптималды басқару жүйелерінің негізгі параметрлері мен сипаттамаларына әсерлерін ескеру тәсілі қарастырылады. Негізгі мәселелердің бірі ретінде масс-спектрометрлердің әртүрлі типтерінің негізгі компоненттерінің бірі болып табылатын катоды қуыс катодты линзалардың және ион көздерінің электронды оптикалық параметрлеріне технологиялық қателердің әсері қарастырылды, бұл олардың негізінде құрастырылған масс-спектрометрлердің ажырату қабілеті мен сезімталдығын, әртүрлі минералдардың, химиялық элементтердің және олардың қоспаларының құрамын талдау саласындағы мүмкіндіктерін анықтайды. Әрі қарай мақала авторлары ұсынған тәсілді әртүрлі экономика салаларында және техникалық кешендер мен технологиялық процестерді басқару жүйелерінің оптималдық көрсеткіштеріне ауытқулардың әсерін талдау мәселелерін шешу үшін қолдануға болатыны көрсетілген. Жұмыстың нәтижелерін әртүрлі типтегі ауытқулардың нақты аспаптар мен технологиялық процестерді басқару жүйелерінің сапасына әсерін талдау және бағалау үшін пайдалануға болады.

Түйін сөздер: минералдар мен қоспалар, талдау, масс-спектрометр, технологиялық ауытқу, оңтайлы басқару, тәсіл, сапа

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МЕТОД УЧЕТА ВЛИЯНИЯ ПОГРЕШНОСТЕЙ НА КАЧЕСТВО АНАЛИТИЧЕСКИХ ПРИБОРОВ И СИСТЕМ ОПТИМАЛЬНОГО УПРАВЛЕНИЯ

Ибраев Алпамыс – доктор физико-математических наук, главный научный сотрудник, Казахстанский университет инновационных и телекоммуникационных систем, Уральск, Казахстан, Казахстанская академия информации и бизнеса, Алматы, Казахстан
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Аннотация. В различных сферах экономики и жизнедеятельности общества, в том числе в нефтегазовой и горнодобывающей отраслях, в геологии, в металлургии и во многих других областях промышленности в настоящее время для обеспечения успешного инновационного развития активно проводятся проектные и исследовательские работы по проектированию и внедрению новых усовершенствованных аналитических приборов и систем управления. При этом на этапах проектирования, изготовления и практического применения аналитических приборов и систем по объективным причинам имеются или возникают погрешности, которые в дальнейшем влияют на качество технологических комплексов или систем управления в целом. В данной работе на основе моделирования и анализа некоторых актуальных проблем рассматривается метод учета влияния погрешностей на основные параметры и характеристики аналитических приборов и систем оптимального управления. В качестве одного из основных проблем рассмотрено влияние технологических погрешностей на электронно-оптические параметры ионных источников, которые строятся на основе катодных линз с полым катодом и являются одним из основных узлов различных типов масс-спектрометров, от разрешающей способности и чувствительности которых в значительной степени зависят возможности в области анализа состава различных минералов, химических элементов и их смесей. Дальше показано, что предложенный авторами статьи метод может быть применен для решения задач по анализу влияния погрешностей на показатели оптимальности систем управления техническими комплексами и технологическими процессами в разных отраслях промышленности и экономики. Результаты работы могут быть использованы для

анализа и оценки влияния различного вида погрешностей на качество конкретных приборов и систем управления технологическими процессами.

Ключевые слова: минералы и смеси, анализ, масс-спектрометр, технологическая погрешность, оптимальное управление, метод, качество

Introduction

In the oil and gas industry, in the mining industry, in geology, in metallurgy and in many other areas of the economy and the life of society, much attention is currently paid to the introduction of innovative technologies and technological systems. Innovative development, as is known, involves active work on the development and implementation of new improved analytical instruments and control systems (Mosichev et al., 2008; Starostin et al., 1997; Dong et al., 2014: 1–8; Ganeyev et al., 2016: 427–444; Lebedev, 2013: 632; Sikharulidze, 2004: 21–30; Ganeyev et al. 2015: 80901–80910; Sanchez et al., 2012: 71–79; Pontryagin et al., 1983: 393). At the same time, at the stages of design, manufacture and practical application of analytical instruments and systems, for objective reasons, there are or occur errors that further affect the quality of technological complexes or control systems as a whole. By belonging to the stages of their origin and manifestations listed above, errors are divided into theoretical, technological and operational. In addition, by origin, errors can also be divided into the following types: subjective, instrumental, external, methodological, errors due to the inadequacy of the model, unforeseen errors. Subjective errors are called errors that depend on the human factor, for example, the qualifications of the operator. Instrumental errors include errors that arise due to the shortcomings of measuring instruments. The causes of such errors are investigated and taken into account when designing new devices. External errors are associated with the influence on the device or processes of physical quantities that are characteristics of the external environment. Methodical errors usually arise due to the shortcomings of the chosen method of analysis or measurements. This is most often due to simplifications, such as various approximations and roundings. Errors caused by the inadequacy of the model used are associated with insufficient correspondence of the model to the objects under study. The adequacy of the object model means that the model sufficiently reflects all the main properties of the object that are of interest for research. Unforeseen errors appear as a result of unforeseen circumstances. Such errors can sometimes occur, for example, when observing artificial satellites of the Earth, when another satellite is mistaken for the satellite under study.

In this paper, we consider a method for taking into account the influence of errors on the main parameters and characteristics of analytical instruments and optimal control systems using some examples, which are given below.

As one of the main problems, let us consider the effect of technological errors on the electron-optical parameters of ion sources, which are built on the basis of cathode lenses with a hollow cathode and are one of the main components of various types of mass spectrometers, the resolution and sensitivity of which largely determine the capabilities in the field of analysis of the composition of various minerals, chemical elements and their mixtures.

Materials and methods

At present, there is a fairly complete theoretical base for studying the properties of various types of elements of electron and ion optics, which allows successful work on the design of ion and electron beam devices and devices with high quality indicators of charged particle focusing (Kel'man et al., 1968: 488; Ibrayev et al., 1981: 22-30; Szilagyi, 1990: 639; Yakushev, 2013: 147–247; Ibrayev et al., 2017: 108–114; Ibrayev, 2015).At the same time, in order to achieve design indicators in their practical implementation, as is known, it is necessary to ensure a sufficient degree of requirements for production technology. In turn, in order to determine the requirements for technology in electron beam instrumentation, it is necessary to study the effect of technological errors on the quality indicators of charged particle focusing in the electronic lenses used. Therefore, we study the effect of technological errors on the ion-optical parameters of an ion source built on the basis of a doubly symmetric cathode lens, the theory and numerical studies of the focusing properties of which were devoted to works (Ibrayev et al., 2017: 108–114; Ibrayev, 2015).

In the Cartesian coordinate system, whose z-axis coincides with the main optical axis and the plane coincides with the lens median plane, the paraxial equations have the form (Ibrayev, 2015).

$$2\Phi\frac{d^2x}{dz^2}+\Phi'\frac{dx}{dz}+\left(\frac{\Phi''}{2}-2f_{KB}\right)x=0, \qquad (1)$$

$$2\Phi\frac{d^2y}{dz^2}+\Phi'\frac{dy}{dz}+\left(\frac{\Phi''}{2}+2f_{KB}\right)y=0. \qquad (2)$$

Here $\Phi=\Phi(z)$ denotes the distribution of the electrostatic potential along the main optical axis, $f_{KB}=f_{KB}(z)$ is the distribution function of the quadrupole component of the lens field, the dashes denote differentiation with respect to z.

Physically, an electronic lens consists of electrodes to which certain potentials are applied and which have certain geometric dimensions. Therefore, inaccuracies or errors in geometric dimensions in the manufacture of the lens, alignment during assembly work, and errors or fluctuations in the potentials (voltages) applied to the lens electrodes constitute the main set of technological errors.

Results and discussions

In general, the distribution of electrostatic potential along the main optical axis can be represented by a function of the following form

$$\Phi = \Phi\left(z, X_\Gamma, Y_\Gamma, Z_\Gamma, U_\Gamma\right), \qquad (3)$$

where $X_\Gamma, Y_\Gamma, Z_\Gamma, U_\Gamma$ denote the sets of values of quantities characterizing the boundary conditions for the Dirichlet problem, and the elements of these sets are the values of specific electrode sizes in measurements of the Cartesian coordinate system and the values of the potentials applied to the electrodes

$$x_{\Gamma i} \in X_{\Gamma}, \qquad y_{\Gamma i} \in Y_{\Gamma}, \qquad z_{\Gamma i} \in Z_{\Gamma}, \qquad u_{\Gamma i} \in U_{\Gamma}. \tag{4}$$

The symbol i in the indices for each of the sets in (4) has its own limit value and varies from 1 to I_1, I_2, I_3, I_4, respectively.

Technological errors will be denoted, taking into account (4), as follows

$$\Delta y_{\Gamma i} = \delta_{2i}, \quad \Delta z_{\Gamma i} = \delta_{3i}, \quad \Delta u_{\Gamma i} = \delta_{4i}. \tag{5}$$

Taking into account (4) and the smallness of the errors in (5), from (3), keeping only the terms of the first order of smallness of the considered small quantities in the expansion in a series, we can obtain

$$\Phi = \Phi(z) + \sum_{i=1}^{I_1} \frac{\partial \Phi}{\partial x_{\Gamma i}} \delta_{1i} + \sum_{i=1}^{I_2} \frac{\partial \Phi}{\partial y_{\Gamma i}} \delta_{2i} + \sum_{i=1}^{I_3} \frac{\partial \Phi}{\partial z_{\Gamma i}} \delta_{3i} + \sum_{i=1}^{I_4} \frac{\partial \Phi}{\partial u_{\Gamma i}} \delta_{4i}. \tag{6}$$

Denoting

$$\frac{\partial \Phi}{\partial x_{\Gamma i}} = \Phi_{1i}, \quad \frac{\partial \Phi}{\partial y_{\Gamma i}} = \Phi_{2i}, \quad \frac{\partial \Phi}{\partial z_{\Gamma i}} = \Phi_{3i}, \quad \frac{\partial \Phi}{\partial u_{\Gamma i}} = \Phi_{4i}, \tag{7}$$

From (6) we get

$$\Phi = \Phi(z) + \sum_{i=1}^{I_1} \Phi_{1i}\delta_{1i} + \sum_{i=1}^{I_2} \Phi_{2i}\delta_{2i} + \sum_{i=1}^{I_3} \Phi_{3i}\delta_{3i} + \sum_{i=1}^{I_4} \Phi_{4i}\delta_{4i} = \Phi(z) + \sum_{n=1}^{4}\sum_{i=1}^{I_n} \Phi_{ni}\delta_{ni}. \tag{8}$$

Similarly, we can decompose

$$f_{KB} = f_{KB}(z) + \sum_{i=1}^{I_1} f_{1i}\delta_{1i} + \sum_{i=1}^{I_2} f_{2i}\delta_{2i} + \sum_{i=1}^{I_3} f_{3i}\delta_{3i} + \sum_{i=1}^{I_4} f_{4i}\delta_{4i} = f_{KB}(z) + \sum_{n=1}^{4}\sum_{i=1}^{I_n} f_{ni}\delta_{ni}, \tag{9}$$

$$x = x(z) + \sum_{i=1}^{I_1} x_{1i}\delta_{1i} + \sum_{i=1}^{I_2} x_{2i}\delta_{2i} + \sum_{i=1}^{I_3} x_{3i}\delta_{3i} + \sum_{i=1}^{I_4} x_{4i}\delta_{4i} = x(z) + \sum_{n=1}^{4}\sum_{i=1}^{I_n} x_{ni}\delta_{ni} \tag{10}$$

$$y = y(z) + \sum_{i=1}^{I_1} y_{1i}\delta_{1i} + \sum_{i=1}^{I_2} y_{2i}\delta_{2i} + \sum_{i=1}^{I_3} y_{3i}\delta_{3i} + \sum_{i=1}^{I_4} y_{4i}\delta_{4i} = y(z) + \sum_{n=1}^{4}\sum_{i=1}^{I_n} y_{ni}\delta_{ni} \tag{11}$$

In the last expressions

$$\frac{\partial f_{KB}}{\partial x_{\Gamma i}} = f_{1i}, \quad \frac{\partial f_{KB}}{\partial y_{\Gamma i}} = f_{2i}, \quad \frac{\partial f_{KB}}{\partial z_{\Gamma i}} = f_{3i}, \quad \frac{\partial f_{KB}}{\partial u_{\Gamma i}} = f_{4i}$$

$$\frac{\partial x}{\partial x_{\Gamma i}} = x_{1i}, \quad \frac{\partial x}{\partial y_{\Gamma i}} = x_{2i}, \quad \frac{\partial x}{\partial z_{\Gamma i}} = x_{3i}, \quad \frac{\partial x}{\partial u_{\Gamma i}} = x_{4i},$$

$$\frac{\partial y}{\partial x_{\Gamma i}} = y_{1i}, \quad \frac{\partial y}{\partial y_{\Gamma i}} = y_{2i}, \quad \frac{\partial y}{\partial z_{\Gamma i}} = y_{3i}, \quad \frac{\partial y}{\partial u_{\Gamma i}} = y_{4i}.$$

Substituting (8) — (11) into equations (1) and (2), grouping similar terms with respect to small values that characterize errors not higher than the first order of smallness, and taking into account the linearity of the paraxial equations, we obtain a number of independent equations

$$2\Phi\frac{d^2x_{ni}}{dz^2}+\Phi'\frac{dx_{ni}}{dz}+\left(\frac{\Phi''}{2}-2f_{KB}\right)x_{ni}=F_{Xni}, \tag{12}$$

$$F_{Xni}=-\left[2\Phi_{ni}x_1''+\Phi_{ni}'x_1'+\left(\frac{\Phi_{ni}''}{2}-2f_{ni}\right)x_1\right]x_k-$$

$$-\left[2\Phi_{ni}x_3''+\Phi_{ni}'x_3'+\left(\frac{\Phi_{ni}''}{2}-2f_{ni}\right)x_3\right]\sqrt{\varepsilon_x},$$

$$2\Phi\frac{d^2y_{ni}}{dz^2}+\Phi'\frac{dy_{ni}}{dz}+\left(\frac{\Phi''}{2}+2f_{KB}\right)y_{ni}=F_{Yni},$$

$$F_{Yni}=-\left[2\Phi_{ni}y_2''+\Phi_{ni}'y_2'+\left(\frac{\Phi_{ni}''}{2}+2f_{ni}\right)y_2\right]y_k- \tag{13}$$

$$-\left[2\Phi_{ni}y_4''+\Phi_{ni}'y_4'+\left(\frac{\Phi_{ni}''}{2}+2f_{ni}\right)y_4\right]\sqrt{\varepsilon_y},$$

where x_1, x_3, y_2, and y_4 are particular linearly independent solutions of paraxial equations x_k, y_k are the coordinates of the charged particle at the moment of its departure from the cathode surface, and $\sqrt{\varepsilon_x},\sqrt{\varepsilon_y}$ characterize the initial energy of the charged particle.

Solutions of equations (12) and (13), which have zero initial conditions, are determined by the method of variation of arbitrary constants from the expressions

$$x_{ni}=x_1\int\frac{x_3}{\sqrt{\Phi}}F_{Xni}dz-x_3\int\frac{x_1}{\sqrt{\Phi}}F_{Xni}dz, \tag{14}$$

$$y_{ni}=y_2\int\frac{y_4}{\sqrt{\Phi}}F_{Yni}dz-y_4\int\frac{y_2}{\sqrt{\Phi}}F_{Yni}dz. \tag{15}$$

Expressions (14) and (15) make it possible to determine the values of aberrational distortions associated with technological errors. Given these values in equations (10) and (11), it is possible to determine specific tolerance values for each type of technological errors.

All the results obtained above can also be used to estimate aberrational distortions associated with technological errors in charged particle sources with axial symmetry of the focusing field. To do this, it is necessary to take the distribution function $f_{KB}=f_{KB}(z)$ of the quadrupole component of the lens field equal to zero. If we accept $f_{KB}=\frac{\Phi''}{4}$, then all formulas obtained above will be valid for two-dimensional planar-symmetric sources of charged particles.

As theoretical errors in the study of the focusing properties of sources of charged particles, one can attribute the neglect in the traditional theory of charged particle optics of aberrations above the third order of smallness.

The method used above to take into account and evaluate the influence of errors on the focusing properties of ion sources is quite universal and can also be applied in problems of analyzing the influence of errors on the optimality indicators of control systems for technical complexes and technological processes in various industries and the economy.

For example, consider the problem of controlling an object, which at each moment of time t is completely described by a finite set of numbers $x_1(t), x_2(t), ..., x_n(t)$ which are called the phase coordinates of the object (Kel'man et al., 1968: 488; Ibrayev et al., 1981: 22-30; Szilagyi, 1990: 639; Yakushev, 2013: 147–247; Ibrayev et al., 2017: 108–114; Ibrayev, 2015; Kiselyov et al., 2007: 270). Let us assume that the law of change of phase coordinates in time is described by a system of ordinary differential equations

$$\dot{x}_i = f_i(t, x_1, x_2, ..., x_n, u_1, u_2, ..., u_m), \tag{16}$$

where i=1,2,...,n, t - time, $\dot{x}_i = \frac{dx}{dt}$ - time derivative of the phase coordinate, u_i- parameters of the control action, $f_i(t, x_1, x_2, ..., x_n, u_1, u_2, ..., u_m)$ - known functions of the arguments indicated in brackets.

For convenience, the reduced system of equations (16) can be written in the generalized (vector) form

$$\dot{x} = f(t, x, u). \tag{17}$$

Equation (17) describes the dynamics of the controlled process. To construct optimal control systems, the concept of control quality criterion J is introduced, which is defined as the following functional

$$J = \int_{t_0}^{t_1} f^0(t, x(t), u(t))\, dt \cdot \tag{18}$$

Here, $f^0(t, x(t), u(t))$ is a function known (given) for a particular task under consideration, x(t) is the trajectory of change (movement) of the controlled parameter over time t, and u(t) is an allowable control action. The initial condition for ()xt is given at the moment of time t_0 in the form $x(t_0) = x_0$.

In practice, the problem of ensuring the quality of optimal control is solved by minimizing the functional J. If there are errors in the initial conditions δ_x and in the values of the control action δ_u, the functional Jmust be considered in a more extended form, compared to (18),

$$J = \int_{t_0}^{t_1} f^0(t, x(t), u(t), \delta_x, \delta_u)\, dt\ . \tag{19}$$

The integrand in expression (19) can be reduced in the first approximation to the form

$$f^0(t, x(t), u(t), \delta_x, \delta_u) = f^0(t, x(t), u(t)) + \frac{\partial f^0}{\partial \delta_x}\delta_x + \frac{\partial f^0}{\partial \delta_u}\delta_u. \tag{20}$$

Then, taking into account (18) - (20), the deviation of the value of the control quality criterion ΔJ, associated with the influence of the noted errors, is determined by the formula

$$\Delta J = \int_{t_0}^{t_1} \left(\frac{\partial f^0}{\partial \delta_x} \delta_x + \frac{\partial f^0}{\partial \delta_u} \delta_u \right) dt \quad . \tag{21}$$

Using (21), one can estimate the absolute and relative values of the errors of the control quality criterion. If these errors are small, they can be neglected, and if they are large, it is necessary to solve specific problems to minimize these errors.

Conclusions

In the conditions of growing demand for an innovative component in all spheres of the economy and the life of society, the need to ensure high accuracy and reliability of analytical instruments, technical means, technological complexes and control systems is certainly increasing. In this article, on specific examples, the problems of accounting for and evaluating the influence of errors on the main parameters and characteristics of analytical instruments and optimal control systems are considered. The method proposed in the paper for taking into account and evaluating negative factors from various kinds of errors can be used in the design of various instruments designed to analyze the composition and properties of substances and their mixtures, as well as in the development of optimal control systems in geology, oil and gas and many other sectors of the economy, industry and manufacturing sector.

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