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Mathematical models and calculation methods for optimally distributed electrical conductivity and reaction surface area of 3D carbon cathodes in galvanic metallization of composite and nanocomposite materials

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ABSTRACT

Introduction. The task of uniformly coating carbon-graphite fibers with metal as a base for composite materials is a pressing issue. Galvanic metallization is preferred due to the ability to control the parameters of the electrochemical system. **Materials and methods.** To determine the effective values of specific electrical conductivity and reactive surface area of a carbon flow three-dimensional electrode (FTE), as well as to identify rational metal electrodeposition modes, mathematical modeling and a combination of calculated and experimental data regarding the feasibility of producing carbon fiber materials (CFM) and FTEs with desired properties are useful. Proper selection of electrolyzer operating modes and parameters allows for intensification of the metallization process and facilitates the production of the desired composites. **Results.** Mathematical models of electrolysis using a CFM were developed in the form of systems of differential equations for the potential distribution functions, polarizing current density, and deposited metal concentration across the electrode thickness. Boundary value problems were formulated. An optimal control problem was posed with control actions in the form of distributed values of the resistivity and specific surface area of the electrode and an optimization criterion – an indicator of the uniformity of metal distribution across the electrode thickness. The solution was based on S.L. Pontryagin's maximum principle and direct selection of control parameters using the equations of the mathematical model. **Discussion.** The proposed mathematical models and methods are consistent with the modern electrochemical theory of metal electrodeposition in FTEs. Accounting for dynamic changes in electrode properties and the metallization process of the carbon-graphite filaments that comprise it expands the applicability of mathematical models to describe real-world electrolysis processes in FTEs and improves the adequacy of the models for real-world physicochemical processes. **Conclusion.** The presented mathematical modeling methods and computational algorithms 1) are used both to study the theoretical principles of electrolysis processes in FTEs and to analyze the properties of actual carbon-graphite material metallization processes; 2) allow one to determine the effective values of the distributed specific electrical conductivity and the reactive surface area of the carbon-graphite material to improve the uniformity of electrodeposition across the TFE thickness and to produce carbon-graphite fibers with desired properties.

KEYWORDS: composite, nanocomposite and carbon-graphite materials, mathematical models and methods, flow three-dimensional electrodes, specific electrical conductivity, reactive surface, optimization

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Математические модели и методы расчета оптимально распределенной электропроводности и реакционной поверхности трехмерных углеродных катодов при гальванической металлизации композиционных и нанокомпозиционных материалов

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АННОТАЦИЯ

Введение. Задача равномерного покрытия металлом углеграфитовых нитей как основы для композиционных материалов является актуальной. Гальваническая металлизация предпочтительна вследствие возможности управления параметрами электрохимической системы. **Материалы и методы.** Для определения эффективных значений удельной электропроводности и реакционной поверхности углеродного проточного трехмерного электрода (ПТЭ), а также выявления рациональных режимов электроосаждения металлов целесообразным является математическое моделирование и сочетание расчетных и экспериментальных данных относительно возможности получения углеродных волокнистых материалов (УВМ) и ПТЭ с заданными свойствами. Правильный выбор режимов работы электролизера и его параметров позволяет интенсифицировать процесс металлизации, способствует получению требуемых композитов. **Результаты.** Разработаны математические модели электролиза на УВМ в виде систем дифференциальных уравнений относительно функций распределения потенциала, плотности поляризующего тока и концентрации осаждающегося металла по толщине ПТЭ. Осуществлена постановка краевых задач. Поставлена задача оптимального управления с управляющими воздействиями в виде распределенных значений удельного сопротивления и удельной поверхности ПТЭ и критерием оптимизации – показателем равномерности распределения металла по толщине электрода. Решение выполнено на основе принципа максимума С.Л. Понтрягина и прямого подбора управляющих параметров по уравнениям математической модели. **Обсуждение.** Предложенные математические модели и методы соответствуют современной электрохимической теории электроосаждения металлов в ПТЭ. Учет динамического изменения свойств электрода и процесса металлизации составляющих его углеграфитовых нитей позволяет расширить применимость математических моделей для описания реальных процессов электролиза в ПТЭ и повышает уровень адекватности моделей реальным физико-химическим процессам. **Выводы.** Представленные методы математического моделирования и вычислительные алгоритмы: 1) используются как для исследования теоретических закономерностей процессов электролиза в ПТЭ, так и для анализа свойств реальных процессов металлизации УВМ; 2) позволяют определять эффективные значения распределенной удельной электропроводности и реакционной поверхности УВМ для повышения равномерности электроосаждения по толщине ПТЭ и получать углеграфитовые волокна с заданными свойствами.

КЛЮЧЕВЫЕ СЛОВА: композиционные, нанокомпозиционные и углеграфитовые материалы, математические модели и методы, проточные трехмерные электроды, удельная электропроводность, реакционная поверхность, оптимизация

ИСТОЧНИКИ ФИНАНСИРОВАНИЯ НАУЧНОЙ РАБОТЫ, РЕЗУЛЬТАТОМ КОТОРОЙ СТАЛА ПУБЛИКАЦИЯ: Исследование выполнено при финансовой поддержке РНФ в рамках научного проекта № 25-21-00135 «Моделирование процессов электрохимической металлизации пористых углеродных композиционных материалов с целью определения эффективных значений распределенных удельной реакционной поверхности и электропроводности проточного трехмерного электрода».

ДЛЯ ЦИТИРОВАНИЯ:
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INTRODUCTION

Carbon fibers, nanofibers, and nanotubes with metals and metallic compounds deposited on their surfaces are used in the creation of supercapacitors, catalysts, composites, and nanocomposite materials [1]. Furthermore, composite materials based on metallized carbon fiber materials (CFMs) are used in high-tech manufacturing for the aviation, space, chemical, medical, and other industries.

When depositing metals on carbon materials, nanotubes, and nanofibers, as well as when directly using them in composite materials, it is important to select a metallization method that ensures good adhesion of the metal to the carbon material surface. The use of various methods of chemical surface activation with strong oxidizing agents, such as concentrated acids, results in significant mass loss of carbon nanomaterials. In this regard, the use of electrochemical methods for depositing metals and their compounds onto the surface of CFMs is of great scientific and practical interest. The potential of using electrochemical metallization methods on CFM electrodes has been demonstrated in various studies, for example, in [2–7].

The monograph [8] publishes the results of experimental studies on the electrochemical modification and deposition of metals on carbon nanofibers (CNF) and nanotubes (CNT), obtained by Professor V.K. Varentsov and his co-workers. The possibility of depositing copper, nickel, and manganese dihydroxide on CNF and CNT by electrolysis and electrosorption from aqueous electrolyte solutions is demonstrated. Micrographs of copper and nickel deposits (Fig. 1) demonstrate the effectiveness of using electrochemical methods for CNT metallization.

It should be noted that sufficient adhesion of the sediment to the surface of the carbon-graphite material is ensured by preliminary functionalization of the CNT surface by electrolysis in a solution of the appropriate electrolyte [8].

A visual analysis of Fig. 1 reveals that copper crystals of varying sizes are present on the CFMs, while they are absent on the carbon-graphite nanotubes. Clearly, the size and structure of the CFMs significantly influence the morphology of the metal deposit, which affects both the kinetics and hydrodynamics of electrode processes. This circumstance necessitates taking into account the specific characteristics caused by the small fiber sizes when mathematically modeling and solving problems of process control in flow three-dimensional electrodes (FTEs) made of CNFs and CNTs.

Carbon-graphite materials in the form of nanofibers and nanotubes are used as electrodes in electrolyzers with flow three-dimensional electrodes, forming a three-dimensional electrochemical system. For theoretical studies and calculations of real processes in flow three-dimensional electrodes, a well-developed framework exists for mathematical modeling of the processes under study, as well as for developing methods and algorithms for calculating real electrochemical processes. The principles of mathematical modeling of electrochemical processes in flow-through three-dimensional electrodes, existing complete mathematical models, their simplifications, methods of their numerical implementation and some calculation results are presented in [8–19].

Mathematical modeling of electrode processes in the FTE from CFM is based on the classical law of material balance of charged particles, which, in the absence of a homogeneous electrochemical reaction, is described by the following system of differential evolutionary parabolic types [20, 21]:

$$\frac{\partial C_i}{\partial t} = -\mathrm{div}\left(z_i \mu_i F C_i \mathrm{grad}(E) + C_i v\right). \qquad (1)$$

Here, the unknown functions are: C_i – the concentration of the i-th electroactive component, $i = 1...n$ and E – the electric field potential; the known functions are: v – the vector of the convective transfer velocity of the electrolyte and the constants z_i, μ_i – the charge and mobility of the i-th electroactive component.

It should be noted that in [20], equation (1) reflects the balance of charged particles in a homogeneous medium, while in [21], model representations are presented that allow the regularities described by equation (1) to be extended to the case of a pseudo-homogeneous medium. It is assumed that at each point of the reaction space, electrode reactions occur involving charged particles present in the bulk-porous system.

Various technological conditions for the operation of electrolyzers with FTE, determined by the tasks set for the deposition of metals on carbon-graphite fibers, determine the paths for further transformation of the modeling system of differential equations (1). The most complete mathematical models describing the electrode processes in FTE from carbon-graphite fibers during the deposition of metals from multicomponent electrolytes in various technological situations are presented in the monograph [8].

Mathematical descriptions of electrochemical processes in FTEs in the form of closed boundary value problems of mathematical physics allow for the formulation of optimization problems as nonlinear programming and optimal mathematical control problems. Thus, work [22] describes an algorithm for calculating the distribution of the specific electrical conductivity of FTEs across the electrode thickness $\kappa(x)$ in the form of so-called simple control, where the selected linear and parabolic dependences $\kappa(x)$ are adopted as the optimal control function. Classical nonlinear programming methods were used to solve the problem. In [23], the problem of calculating $\kappa(x)$ was posed as an optimal mathematical programming problem and solved using L.S. Pontry-

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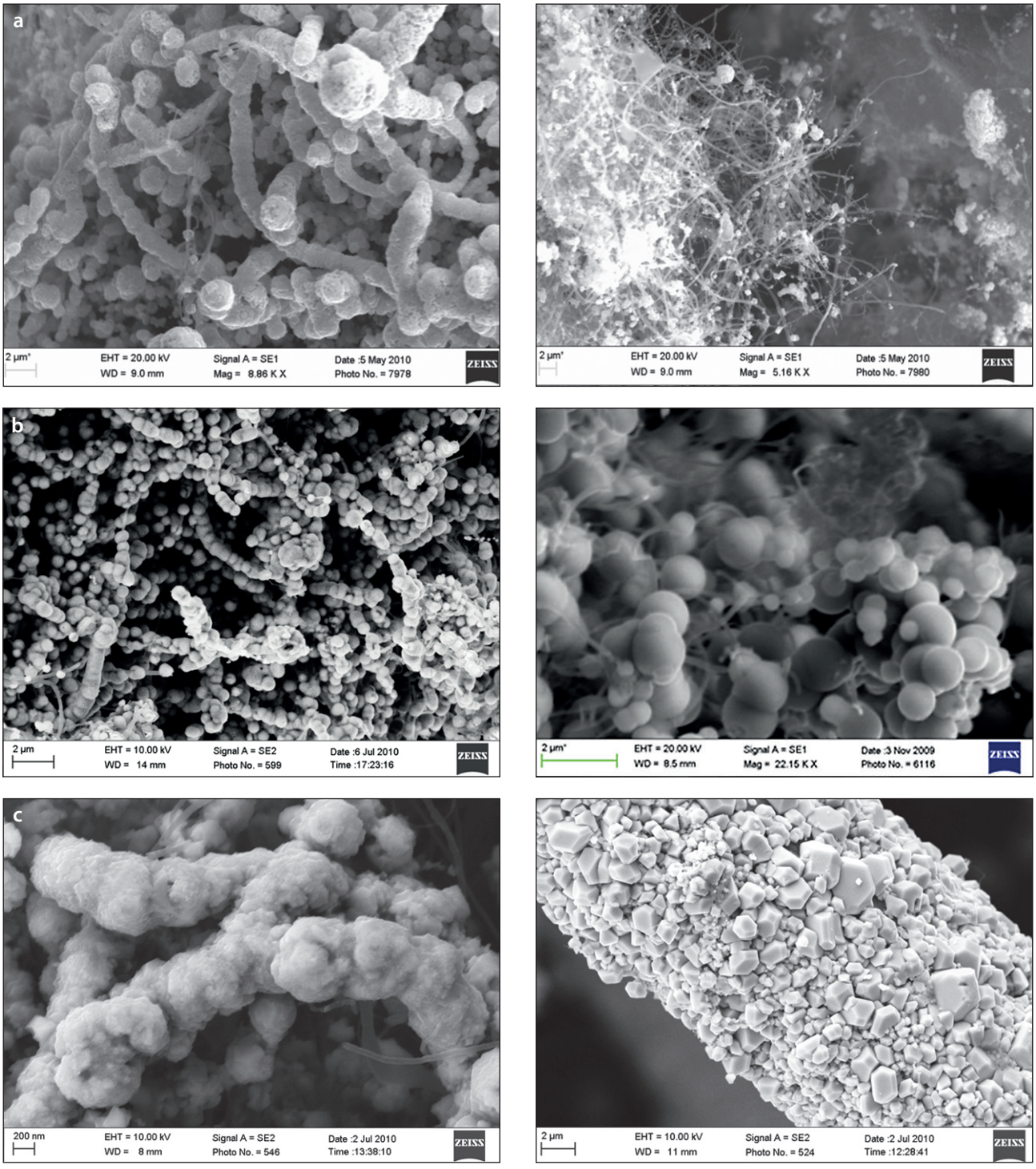

Fig. 1. Nanotubes with copper (a), nickel (b) deposits; CFM with electrolytically deposited copper (c)

agin's well-known maximum principle. The maximum principle was also applied to the problem of calculating the optimal distribution of the specific reaction surface area from the coordinate across the electrode thickness $S_v(x)$ [19].

This paper proposes an extension of the results for determining optimal operating conditions for electrolyzers with CFM-based FTEs. When the control variables are both $\kappa(x)$ and $S_v(x)$, the functional representing the optimal control criterion in L.S. Pontryagin's maximum principle depends on two distributed variables, significantly complicating the problem when formulating it and, especially, when implementing the maximum principle numerically. In addition, the analysis of experimental

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data arrays corresponding to the properties of CFM of various brands shows that in some cases there is a correlation between the value of specific electrical conductivity κ and the specific reaction surface $S_v(x)$, and, therefore, the problem of jointly determining the optimal values of $\kappa(x)$ and $S_v(x)$ is relevant.

MATERIALS AND METHODS

Analysis of carbon fiber material parameters

The influence of distributed values of $\kappa(x)$ and $S_v(x)$ on the uniformity of the distribution of the metal coating of the carbon-graphite material has been studied, for example, in [19, 22, 23]. It has been shown that with the correct selection of the sequence of carbon-graphite materials of different grades in the sections of the FTE, it is possible to achieve a significant improvement in the distribution of the metal across the thickness of the FTE. This circumstance necessitates considering the properties of the most commonly used grades of carbon-graphite material from the point of view of the formation of FTE with distributed properties, in particular $\kappa(x)$, $S_v(x)$ and the porosity of the material $\varepsilon(x)$.

The values of the parameters of the CFM – κ, S_v, ε – can be found in the works of V.K. Varentsov, A.A. Konkin, A.S. Fialkov, I.N. Ermolenko and other authors [1, 24–28]. The main characteristics of some CFM are presented in Table 1.

It should be noted that the value of the specific reaction surface of carbon-graphite materials can be determined by the so-called gravimetric and electrochemical methods [24, 25], between which there is a significant correlation [29]. However, it was also shown there that a significantly more significant relationship is observed between the value of the specific reaction surface, the radius of the carbon-graphite fiber and the porosity of the carbon-graphite materials. Based on this, to determine the specific surface of carbon-graphite materials for which data on S_v are not available in the literature, we used a linear regression equation with a high correlation coefficient [19]:

$$S_v = 3066.93 - 574.911r + 24.567\varepsilon.$$

Furthermore, when filling out Table 1, we assumed that S_v doubles upon compression of the CFM. This assumption is likely true for the materials under consid-

Table 1. Properties of various grades of CFM

No.	Material	*r*, μm	S_v, cm^{-1}	κ, Siemens/cm	ε
1	VNG-50/VNG-50*	6.0	265/530	1.3/2.6	0.92/0.84
2	VNG-30/VNG-30*	5.5	160/320	0.90/0.33	0.96/0.92
3	VINN-250/VINN-250*	4.5	280/560	0.1/0.4	0.97/0.94
4	NTM-200/NTM-200*	5.0	216/432	0.07/0.4	0.96/0.92
5	NTM-100/NTM-100*	5.4	220/440	0.03/0.12	0.96/0.92
6	Mtilon/Mtilon*	5.1	270/540	0.13/0.5	0.94/0.88
7	VVP-66-95/VVP-66-95*	4.7	255/510	0.006/0.05	0.96/0.92
8	FRN/FRN*	5.0	125/250	0.001/0.005	0.98/0.96
9	KNM/KNM*	6.1	160/320	0.009/0.03	0.98/0.96
10	VINN-150/VINN-150*	5.0	220/440	0.05/0.16	0.92/0.84
11	KSS/KSS*	4.5	501/1000	0.1/0.2	0.89/0.78
12	Uglen/Uglen*	5.1	240/480	0.05/0.13	0.95/0.90
13	Gralen/Gralen*	4.9	260/520	0.1/0.4	0.96/0.92
14	NT-1/NT-1*	6.2	165/330	0.001/0.02	0.90/0.80
15	NT-2/NT-2*	6.2	165/330	0.003/0.014	0.90/0.80
16	ANM/ANM*	6.1	180/360	0.01/0.12	0.96/0.92
17	TVSh/TVSh*	4.6	780/1560	0.16/0.4	0.91/0.82
18	TVSh/TVSh*	5.0	220/440	0.45/1.5	0.85/0.70
19	LVIK-95/LVIK-95*	6.0	270/540	0.26/0.87	0.83/0.66
20	LG-50/LG-50*	3.8	150/300	0.02/0.09	0.76/0.52
21	LG-30/LG-30*	3.7	180/360	0.64/2.1	0.78/0.56
22	LG-10/LG-10*	3.4	170/340	0.44/1.4	0.77/0.54
23	Carbonactalone-TK-24	3.5	1032/2064	0.41	0.87/0.74
24	KBN-24	3.5	285	0.61	0.87/0.74
25	B-1	3.0	282	0.55	0.93/0.86
26	B-2	3.0	537	0.016	0.90/0.80

* – materials obtained by compressing a material in a free state by half.

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eration, as they all have very high porosity, and therefore, significant fiber "sticking" under compression is unlikely.

The value of the porosity coefficient during compression of the CFM can be easily recalculated using the formula $\varepsilon = 1 - 2V_M/V$, where V_M is the volume occupied by the CFM fibers in a unit volume V of the electrode; $r = 2(1 - \varepsilon)/S_v$ – radius of the fiber, provided that each individual fiber is a cylinder of radius r.

A simple visual analysis of the data in Table 1 shows that various grades of CFM can be used to assemble composite materials with various properties, for example, with specific electrical conductivity $\kappa(x)$ or specific reactive surface area $S_v(x)$ distributed across the thickness in the form of linear, parabolic, and other dependences. The ability to form such composite materials facilitates the formulation and solution of problems aimed at producing composite materials with specified properties through galvanic metallization.

Another method for producing carbon-graphite fiber cathodes with distributed properties across the thickness of the FTE, as already noted, is the electrochemical functionalization of the carbon-graphite fiber cathodes in various electrolytes, for example, in sulfuric acid solutions [8]. Such processing allows, in some cases, the production of carbon-graphite fiber cathodes with specified characteristics, for example, with distributed specific conductivity of the required profile.

All of the above circumstances determine the relevance and possibility of developing methods of mathematical modeling, calculation and optimization of galvanic metallization processes of CFM in order to determine the conditions necessary for the creation of composite and nanocomposite materials with the required characteristics.

Mathematical model

In our previously published works [8, 17, 19, 23, 24, 30, 31], we examined in detail the methods for modeling electrochemical processes in FTE in various technological situations, with and without taking into account the reactions accompanying the main process of extracting metals and their alloys, such as the release of hydrogen gas, the oxygen electrode reaction, taking into account the multi-stage deposition process, etc. The mathematical model presented in this paper differs from previously obtained and published models in that it takes into account the distribution of both the specific electrical conductivity and the specific reactive surface area of the electrode across the thickness of the FTE. Since the derivation of the mathematical model under the given conditions is fundamentally no different from previously published methods for obtaining modeling equations, in this publication we present the resulting equations obtained by transforming the fundamental system of differential equations (1), taking into account assumptions and simplifications similar to those used in the development of earlier models.

We will adopt the following notation:

$$a = \frac{zF}{RT}; b = \frac{j_0}{zFK_m}; d = \frac{1}{\nu zF}; g = \frac{1}{\kappa_T} + \frac{1}{\kappa_G};$$

$$u_1 = d\kappa_T(x)/dx; u_2 = S_v(x);$$

$$y_1 = E(x); y_3 = C(x). \quad (2)$$

The system of equations modeling the distribution of the electrochemical process by thickness x of the FTE can be written as:

$$\frac{dy_1}{dx} = y_2 = f_1(y_1, y_2, y_3, u_1, u_2);$$

$$\frac{dy_2}{dx} = \frac{-\kappa_G u_1(x)}{\kappa_T(\kappa_T+\kappa_G)} y_2 + u_2(x)\left(\frac{1}{\kappa_T} + \frac{1}{\kappa_G}\right) j_S(x) =$$

$$= f_2(y_1, y_2, y_3, u_1, u_2);$$

$$\frac{dy_3}{dx} = -\frac{u_2(x)}{\nu zF} J_S(x) = f_3(y_1, y_2, y_3, u_1, u_2);$$

$$\frac{dy_1}{dx}(0) = \frac{I}{\kappa_T}; \quad \frac{dy_1}{dx}(L) = -\frac{I}{\kappa_G}; y_3(0) = C_0;$$

$$J_S(x) = j_0 \frac{e^{\alpha zF((E-\phi_R)/RT} - e^{(\alpha-1)zF(E-\phi_R)/RT}}{1+j_0 e^{\alpha zF(E-\phi_R)/RT}/zFK_m C}. \quad (3)$$

Here S_v is the specific reaction surface, J_S is the polarizing current density in the metal; I is the density of the overall current supplied to the FTE; L is the thickness of the FTE; C_0 is the concentration of metal ions in the volume of electrolyte supplied to the FTE; κ_T and κ_G are the specific electrical conductivity of the solid and liquid phases of the system; ϕ_R, α, z are the equilibrium potential, transfer coefficient and valence of the discharging ion of the electrode reaction, x is the coordinate along the thickness of the electrode. The dimensions of the units of physical quantities correspond to the International System of Units.

Solution Method

Method and Algorithm for Integrating Modeling Equations

In our works [32, 33], the instability of system (3) with respect to both the initial conditions and the right-hand side was demonstrated. These proven assertions imply, firstly, the limited applicability of finite-differ-

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ence methods for solving system (3) and, secondly, the necessity of controlling the solution of the problem by numerical methods. When solved by finite-difference methods, the system of ordinary differential equations (ODE) (3) is transformed into a cumbersome, ill-conditioned system of nonlinear algebraic equations, the solution of which requires the use of regularizing computational algorithms, which is difficult for their numerical implementation.

System (3) is a two-point boundary value problem, the most effective method for solving which is the "trial and error" method, when at the first stage, some missing initial value $y_1(0) = y_0$ is specified on the left boundary of the integration interval of the system, as a result of which problem (3) is transformed into a classical Cauchy problem for an ODE system, for the solution of which one can use known integration methods, for example, the Runge – Kutta method and its modifications. After solving the Cauchy problem, the calculated value $dy_1/dx\ (L) = y_1^0$ is compared with the given value $dy_1/dx\ (L) = -I/\kappa_G$, and if they do not correspond sufficiently, the value y_0 is adjusted using some accepted computational algorithm (for example, the direct search method). The search for y_0 ends when the specified accuracy of coincidence between the values y_1^0 and $-I/\kappa_G$ is achieved.

For the numerical implementation of the described method, we carried out studies to determine the initial value y_0 so that it approximates the true, unknown value $y_1(0)$ with a certain accuracy. By simplifying and transforming system (3), similarly to how we did it in [33], we obtained the expression:

$$y_1(0) \approx \frac{2}{\alpha a} Ln\left(\frac{\alpha a J}{2\kappa_T^2 g S v j_0}\right). \quad (4)$$

We used the calculated $y_1(0)$ as the initial value of y_0 when implementing the trial-and-error method, which significantly reduced the calculation volume and increased the accuracy.

Numerous calculations of the distribution of electrochemical functions–electrode potential, polarizing current density, electroactive substance concentration, and other distributed functions – using various methods (Euler, Runge – Kutta, Merson, Adams) showed that the curves corresponding to the solution functions undergo the greatest changes at points adjacent to the current lead and the outer boundary of the bulk-porous cathode (Fig. 2). This led to the use of calculation methods using integration grids with an unequal distribution of nodes: with smaller steps at the edges of the integration interval and larger ones in the central part.

Numerical experiments have shown that the fourth-order Runge – Kutta method on an integration grid with a properly selected non-uniform grid of integration nodes is the most economical method in terms of the number

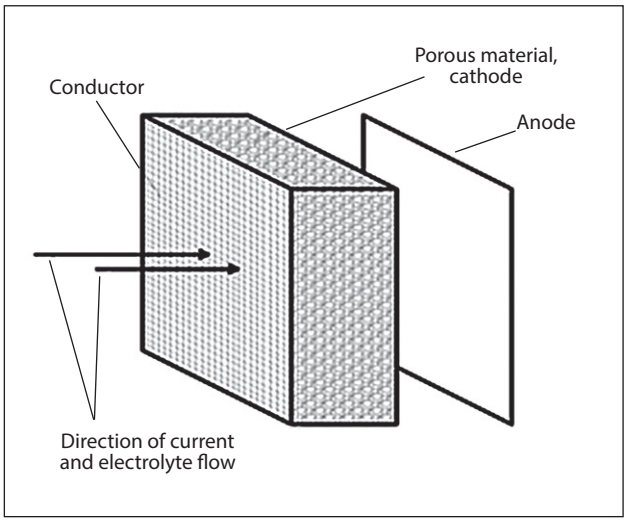

Fig. 2. Schematic representation of the FTE with parallel directions of the current vectors supplied to the electrode and the electrolyte flow rate

of computational operations while maintaining sufficient solution accuracy.

For the numerical implementation of the method for solving the ODE system (3), a software package based on problem-oriented computational procedures [34] was developed. The decomposition of its components into independent components, implemented using the Parallel Programming Library, significantly improved the computational performance.

Methods for solving process distribution optimization problems in FTEs

To calculate optimally distributed values of specific electrical conductivity $\kappa(x)$ and specific reaction surface area $S_v(x)$ across electrode thickness x, ensuring the best uniformity of distribution of the CFM metal coating, two complementary methods were used, each of which has independent value and can be used in conjunction with the other:

1) Determination of the type of dependencies and values of distributed values of specific electrical conductivity $\kappa(x)$ and specific reaction surface $S_v(x)$ from the electrode coordinate x using the classical maximum principle of L.S. Pontryagin [19].

2) Calculation of the best distributed values $\kappa(x)$ and $S_v(x)$ according to the uniformity criterion in the form of so-called simple control, in the form of elementary functions: constant, linear, quadratic forms and their combinations.

To implement the first method, the optimization problem was formulated as an optimal mathematical control problem: an optimization criterion was defined, an ODE system conjugate to this criterion was constructed, and, in accordance with L.S. Pontryagin's

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maximum method, the dependence of the optimization criterion on the type of dependencies of the distributed values $\kappa(x)$ and $S_v(x)$ was analyzed, and their optimal forms were determined.

In implementing the second solution method, the control functions were represented as parabolic forms $\kappa(x) = c_1 + b_1x + a_1x^2$, $S_v(x) = c_2 + b_2x + a_2x^2$, whose unknown coefficients c_i, b_i, a_i, $i = 1.2$, were calculated using a combination of coordinate and gradient descent methods. Depending on the need to determine the accuracy of the problem solution, the obtained results can be used as initial results for solving computational procedures using L.S. Pontryagin's maximum method. Corresponding computer procedures have been written to implement the optimization.

Investigation of the control functions κ(x) and $S_v(x)$ using L.S. Pontryagin's classical maximum principle

The formulation of the problem of optimizing the distribution of specific electrical conductivity and specific reaction surface consists of finding such a vector function $u = (u_1, u_2)$, $u_1(x) = d\kappa_T(x)/dx$, $u_2(x) = S_v(x)$, which would satisfy the system of differential equations (2), (3) and provide a minimum to the functional

$$\sigma(u) = \int_0^L \left(\frac{I}{L} - J_S(u_1(x), u_2(x), y_1(x), y_2(x), y_3(x))\right)^2 dx. \quad (5)$$

The numerical values of functional (5) reflect the uniformity of the current density distribution across the thickness of the FTE, and the smaller these values, the closer the distributed current density is to its average value, and therefore to an absolutely uniform distribution on the FTE.

According to L.S. Pontryagin's maximum principle, in order for the solution to problem (2), (3) $\{u_1(x), u_2(x), y_1(x), y_2(x), y_3(x)\}$ to correspond to the optimal mathematical control $\{u_1^*(x), u_2^*(x)\}$, minimizing functional (5), it is necessary to have a solution to the system of differential equations (6), adjoint to system (2), (3) with respect to the newly introduced functions $\varphi_0, \ldots, \varphi_3$, adjoint to the functions $y_i(x)$, with certain boundary conditions (6):

$$\frac{d\varphi_i}{dx} = -\sum_{j=0}^{j=3} \varphi_j \frac{\partial f_j}{\partial y_i}, \quad i = 0, \ldots, 3;$$

$$\varphi_0(0) = 1; \varphi_1(L) = \varphi_2(L) = \varphi_3(L) = 0. \quad (6)$$

In this case, the system (2), (3) is supplemented by an equation for the function $y_0(x)$, satisfying the relations

$$\frac{dy_0}{dx} = \left(\frac{I}{L} - J_S(x, u_1, u_2)\right)^2 =$$

$$= f_0(y_0, y_1, y_2, y_3, u_1, u_2), \quad y_0(0) = 0. \quad (7)$$

The problem of finding optimal mathematical control consists of determining the minimum of the functional $\sigma(u)$ for the vector $u = (u_1, u_2)$:

$$\min \left[\sigma(u_1(x), u_2(x)) = \int_0^L \left(\frac{I}{L} - J_S(u_1(x), u_2(x), y_1(x), y_2(x), y_3(x))\right)^2 dx\right]. \quad (8)$$

with restrictions:

$$\begin{cases} \frac{dy_i}{dx} = f_i(y_1, y_2, y_3, u_1, u_2); \quad y_0(0) = 0; \\ \frac{dy_1}{dx}(0) = \frac{I}{\kappa_T}; \frac{dy_1}{dx}(L) = \frac{I}{\kappa_G}; y_3(0) = C_0; \\ \frac{d\varphi_i}{dx} = -\sum_{j=0}^{j=3} \varphi_j \frac{\partial f_j}{\partial y_i}; \quad \varphi_0(0) = 1; \\ \varphi_1(L) = \varphi_2(L) = \varphi_3(L) = 0; i = 0, \ldots, 3. \end{cases} \quad (9)$$

The type of functions $f_i(y_1, y_2, y_3, u_1, u_2)$ is determined by the relations in equations (3), (6):

$$f_0(y_1, y_2, y_3, u_1, u_2) = \left(\frac{I}{L} - J_S(x, u_1, u_2)\right)^2;$$

$$f_1(y_1, y_2, y_3, u_1, u_2) = y_2;$$

$$f_2(y_1, y_2, y_3, u_1, u_2) = \frac{-\kappa_G u_1(x)}{\kappa_T(\kappa_T + \kappa_G)} y_2 +$$

$$+ u_2(x)\left(\frac{1}{\kappa_T} + \frac{1}{\kappa_G}\right) j_S(x);$$

$$f_3(y_1, y_2, y_3, u_1, u_2) = -\frac{u_2(x)}{vzF} J_S(x);$$

$$J_S(x) = j_0 \frac{e^{\alpha zF((y_1 - \phi_R)/RT} - e^{(\alpha-1)zF(y_1 - \phi_R)/RT}}{1 + j_0 e^{\alpha zF(y_1 - \phi_R)/RT}/zFK_m y_3}. \quad (10)$$

The system of differential equations (9) involves components of the Jacobian matrix of the vector function $f = (f_1, f_2, f_3, f_4, f_5)$:$[\partial f_j/\partial y_i]$, the calculation of which is not very difficult, but the analytical expressions for some components are quite cumbersome and are not presented in this paper.

The so-called Hamiltonian function, defined by the formula, is involved in solving the optimal control problem.

$$H(x, y_0(x), \ldots, y_4(x), \varphi_0(x), .., \varphi_4(x), u) =$$

$$= \sum_0^3 \varphi_i(x, y_0, .., y_4, u_1, u_2) f_i(x, \varphi_0, .., \varphi_4, u). \quad (11)$$

For the Hamiltonian function, according to the maximum principle, the optimal control $(u_1^*(x), u_2^*(x))$ is a stationary point (at which the partial derivatives of the function $H(u_1, u_2)$ vanish).

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Thus, solving the problem of determining the optimal distributed values of $\kappa(x)$ and $S_v(x)$ using the maximum principle reduces to minimizing the functional (11) under differential constraints (9). We provide a brief description of the algorithm for numerically implementing the maximum principle for our problem.

Let us assume that at the k-th iteration the values of the control vector function $u^k(x) = u_{1,1}{}^k, u_{1,2}{}^k, ..., u_{1,n}{}^k, u_{2,1}{}^k, u_{2,2}{}^k, ..., u_{2,n}{}^k$ are determined. Here the second value of the subscript corresponds to the coordinate x_j ($j = 1, n$) along the electrode thickness; the (k+1)-th iteration is performed according to the following scheme.

1) The sequence $u_{1,1}{}^{k+1}, u_{1,2}{}^{k+1}, ..., u_{1,n}{}^{k+1}, u_{2,1}{}^{k+1}, u_{2,2}{}^{k+1}, ..., u_{2,n}{}^{k+1}$ is calculated using the formula:

$$Fu_{i,j}^{k+1} = u_{i,j}^{k} + \propto \left(\frac{\partial H}{\partial u_i}\right)_j^k;\ i = 1,2;\ j = 1,\ldots,n, \quad (12)$$

Where $\propto$ is a numerical parameter whose value is chosen based on computational experience, typically $\propto \leqslant 1$. The vector grad $(H(u_1, u_2)) = (\partial H/u_1, \partial H/u_2)$ can be calculated both analytically, with certain simplifications, and numerically.

2) After calculating $u^{k+1}(x)$ we solve the system of equations consisting of the first group of equations (9). A numerical method based on the Runge – Kutta method is convenient for integrating the system.

3) Defining the functions y_i^{k+1} allows us to integrate the second group of equations in system (9), resulting in the numerical values of the functions φ_i^{k+1}.

4) We calculate the functional $\sigma(u_1{}^{k+1}, u_2{}^{k+1})$ and compare it with $\sigma(u_1{}^k, u_2{}^k)$. If the condition $\sigma(u_1{}^{k+1}, u_2{}^{k+1}) \leqslant \sigma(u_1{}^k, u_2{}^k)$ is met, then proceed to step 5. Otherwise, in formula (12), we decrease the value of $\propto$ and repeat the calculation.

5) Using the found functions y_i^{k+1} and φ_i^{k+1}, we calculate the function H using formula (11).

6) Using expression (12), we find $u_1{}^{k+2}, u_2{}^{k+2}$. If the values of these functions at all points $x_j, j = 1, ..., n$, along the electrode thickness differ from the values $u_1{}^{k+1}, u_2{}^{k+1}$ by a value greater than a certain specified value that determines the accuracy of the solution, the computational process continues according to the same scheme, points 1) – 6), otherwise the solution process ends, and the vector function $u^* = (u_1{}^*(x), u_2{}^*(x)) = (u_1{}^{k+2}, u_2{}^{k+2})$ is taken as the optimal control.

The derivative of the distributed specific electrical conductivity function $u_1{}^*(x) = d\kappa_T(x)/dx$ and the distributed specific surface area function $u_2{}^*(x) = S_v(x)$, obtained as a result of calculations according to points 1–6, determine the solution to the stated optimization problem.

It should be noted that exact solutions to the optimal control problem using the maximum principle method may prove difficult to implement when designing a FTE, for example, due to the lack of an appropriate CFM constituting a volumetric porous cathode, or due to an excessively complex optimal conductivity profile or specific reaction surface area of the FTE being designed. In this case, solving the problem in the form of so-called simple control, where the profiles of the control actions being optimized are not overly complex elementary curves, can be useful.

Obviously, the accuracy and speed of solving an optimization problem using L.S. Pontryagin's maximum principle is largely determined by the proximity of the initial values of the control action $u_1{}^0, u_2{}^0$ to the solution.

To solve the optimization problem in the form of simple control and to calculate the initial values of the control functions with their subsequent use in implementing the maximum principle, the method described below is proposed.

A method for calculating the distributed values of κ(x) and S_v(x) as quadratic forms

We represent the control functions as parabolas $\kappa(x) = c_1 + b_1x + a_1x^2$, $S_v(x) = c_2 + b_2x + a_2x^2$ with initially unknown coefficients c_i, b_i, a_i, $i = 1,2$. Note that this representation of $\kappa(x)$ and $S_v(x)$ allows us to find effective controls, in addition to parabolic ones, in the form of increasing and decreasing linear functions and in the form of constants.

The proposed algorithm for calculating the effective coefficients c_i, b_i, a_i, $i = 1,2$ is as follows.

1. Determining the initial values of the unknown coefficients. The initial values of the coefficients c_i,b_i, a_i are determined by enumerating possible and most realistic variants of the unknown coefficient values. The subsequent computational procedure consists of sequentially finding each of the sets c_1,b_1, a_1 and c_2,b_2, a_2 on numerical grids in which the horizontal axis is the coordinate along the cathode thickness, and the vertical axis corresponds to the functions $\kappa(x)$ or $S_v(x)$. The vertex of the desired parabola is placed sequentially at each grid point, and the values of b_i and a_i are calculated according to the value of c_i.

2. The found values c_i,b_i, a_i are refined by the gradient search method according to the criterion of the best uniformity of the current density distribution across the thickness of the FTE (8). In this case, at each iterative step of the gradient search, the Cauchy problem for the system of differential equations (2), (3) is solved by the previously proposed numerical method based on the Runge – Kutta method with an adaptive integration step. The parabolic functions $\kappa(x) = c_1 + b_1x + a_1x^2$ and $S_v(x) = c_2 + b_2x + a_2x^2$ are determined in the following order.

– Given the initial function $S_v(x)$, the optimal coefficients of the parabola $\kappa(x) = c_1 + b_1x + a_1x^2$ are calculated.
– Given the found parabolic form $\kappa(x)$, the optimal coefficients of the parabola $S_v(x) = c_2 + b_2x + a_2x^2$ are calculated.

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– Given the found function $S_v(x)$, the optimal coefficients of the parabola $\kappa(x)$ are refined.
– For the newly found function $\kappa(x)$, the coefficients of $S_v(x)$ are refined.
– The calculation algorithm is then carried out according to the same scheme until the specified accuracy is met.

Note that the described computational scheme, in addition to its relative simplicity in algorithmization, has another significant advantage: the ability to determine all local minima of the objective function.

An example of calculating the distributed values of κ(x) and $S_v(x)$ as quadratic forms

Calculations of optimally distributed specific electrical conductivity and reaction surface $\kappa(x) = c_1 + b_1x + a_1x^2$ and $S_v(x) = c_2 + b_2x + a_2x^2$ were carried out at the values of electrochemical parameters and constants characteristic of the process of copper electrodeposition on FTE from a sulfuric acid electrolyte of the composition (g/l): Cu – 0.16; H_2SO_4 – 25; $(NH_4)_2SO_4$ – 80 [8] on the FTE cathode with a thickness of 0.6 cm, at a current density of 150 A/m², at a volumetric flow rate of electrolyte of 0.1 ml/(s·cm²).

The following limits for the change in electrical conductivity and reaction surface were adopted: $0.1 \leqslant (x) \leqslant 0.6$ (S/cm), $200 \leqslant S_v(x) \leqslant 300$ (cm²/cm³). The optimal quadratic distribution of the function $\kappa(x)$ was found in the form of a parabola with upward branches and the apex in the central part of the electrode, and the optimal distribution of the function $S_v(x)$ with the found distribution of $\kappa(x)$ was a parabola with downward branches. The uniformity index $(\max E(x))/(\min E(x) = 1.18)$. For comparison, for parabolic distributions $\kappa(x)$ and $S_v(x)$, respectively, branches down and branches up $\max E(x))/(\min E(x) = 1.22$, branches up and branches up $\max E(x))/(\min E(x) = 1.20$, branches down and branches down $E(x))/(\min E(x) = 1.44$. The known best distribution of $\kappa(x)$ and $S_v(x)$, found experimentally [36], corresponds to the case when $\kappa_T(x)$ is an increasing curve within the same range of variation, and $S_v(x)$ is a parabola with downward branches within the same range of variation, which indicates good agreement between the calculated and experimental results.

Study of the properties of control functions κ(x), $S_v(x)$ using the maximum principle according to model (1), (2) using natural assumptions and simplifications

Consider the method and solutions to problems of optimizing the distribution of distributed resistance and a separate barrier surface when implementing some assumptions regarding the technological characteristics of the galvanic metallization process of FTE with the aim of expanding the metal coating of the CFM and boundaries with such simplifications of the mathematical model (2), (3) and the formulation of control problems (2), (3), (5).

Firstly, since the galvanic coating of the CFM metal is carried out without applying high values of electric current to the electrode, it can be assumed that there is no abrupt change in the specific electrical conductivity of the electrode. This means that the value of $(d\kappa_T/dx)(x)$ at all points with the x-coordinate across the thickness of each electrode layer is insignificant $((d\kappa_T/dx) \sim 0)$ and the function $\kappa(x)$ can be considered a piecewise linear form. Consequently, the first term in the second equation of system (3) and the first term in the third equation of group (10) can be neglected, which significantly simplifies the mathematical model.

Secondly, in the case under consideration, the decrease in the concentration of the deposited metal ions during the passage of a unit volume of electrolyte through the flow electrode can be considered insignificant. In this case, $(dC/dx)(x) \sim 0$ for all x, which leads to the possibility of not considering the third equation in the mathematical model (3) $(dy_3/dx = -(u_2(x)/vzF)\, J_S(x) = f_3(y_1, y_2, y_3, u_1, u_2) = 0)$.

In addition, we assume that the dependence of the polarizing current density $J_S(x)$ on the potential $E(x)$ can be approximated by a linear form and, therefore, the optimization criterion can be represented as:

$$F\sigma\left(u_1(x), u_2(x)\right) = \int_0^L abs\left(E_{cp} - E\left(u_1(x), u_2(x), y_1(x), y_2(x), y_3(x)\right)\right) dx. \quad (13)$$

In this case, the control action $u_1(x)$ is taken to be the specific electrical conductivity function $\kappa(x)$: $u_1(x) = \kappa(x)$.

These assumptions lead to significant simplifications of the mathematical model (2), (3), and, consequently, of system (9), (10):

Assuming that the optimal control $u_1(x)$, $u_2(x)$ has been found, and the distribution of the polarizing current $J_S(x)$ can be represented by some average value, then system of equations (9), (10) takes the form:

$$\begin{cases} \frac{dy_0}{dx} = \left|E(x) - E_{cp}\right| = f_0\left(y_1, y_2, y_3, u_1, u_2\right); \\ \frac{dy_1}{dx} = y_2 = f_1\left(y_1, y_2, y_3, u_1, u_2\right); \\ \frac{dy_2}{dx} = u_2(x)\left(\frac{1}{u_1(x)} + \frac{1}{\kappa_G}\right) J_S(x) = f_2\left(y_1, y_2, y_3, u_1, u_2\right); \\ \varphi_0(x) = 1; \\ \frac{d\varphi_1}{dx} = \mathrm{sign}\left(E - E_{cp}\right); \\ \frac{d\varphi_2}{dx} = -\varphi_1; \\ y_0(0) = 0;\ y_2(0) = \frac{1}{u_1(0)} I; \\ y_2(L) = \frac{1}{\kappa_G} I;\ \varphi_0(0) = 1; \\ \varphi_1(L) = \varphi_2(L) = 0. \\ J_S(x) = j_0 \frac{e^{\alpha zF((y_1 - \phi_R)/RT} - e^{(\alpha-1)zF(y_1 - \phi_R)/RT}}{1 + j_0 e^{\alpha zF(y_1 - \phi_R)/RT}/zFK_m C_0}. \end{cases} \quad (14)$$

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From system (14) it is easy to obtain solutions $\varphi_1(x) = (x - L)\,\mathrm{sign}(E - E_{cp})$, $\varphi_2(x) = 1/2(x - L)^2\,\mathrm{sign}(E - E_{cp})$ and an expression for the Hamilton function for problem (13), (14):

$$H(x, y_0(x), \ldots, y_2(x), \varphi_0(x), \ldots, \varphi_2(x), u_1, u_2) =$$
$$= \sum_0^2 \varphi_i(x, y_0, \ldots, y_4, u_1, u_2) f_i(x, \varphi_0, \ldots, \varphi_4, u) =$$
$$-\left|E(x) - E_{cp}\right| + (x - L)\mathrm{sign}\left(E - E_{cp}\right)y_2 +$$
$$+\frac{1}{2}(x - L)^2\mathrm{sign}\left(E - E_{cp}\right)u_2\left(\frac{1}{u_1} + \frac{1}{\kappa_G}\right)J_S(x). \qquad (15)$$

According to the maximum principle, the smaller the numerical value of the Hamiltonian function at each minimization step, the closer the control vector to its optimal value. Analysis of expression (15) regarding the dependence of the Hamiltonian function on the control actions $u_1(x)$, $u_2(x)$ shows that the value of $H(x, u_1, u_2)$ at $\mathrm{sign}(E - E_{cp}) = 1$ (that is, when $E - E_{cp} > 0$) will be the smaller, the smaller the value of $u_2(x) = S_v(x)$ and the larger $u_1(x) = \kappa(x)$. And vice versa, when $E - E_{cp} > 0$ and $\mathrm{sign}(E - E_{cp}) = -1$, the value of $H(x, u_1, u_2)$ will be the smallest at maximum values of $u_2(x) = S_v(x)$ and minimum values of $u_1(x) = \kappa(x)$.

From the theory of distribution of the electrochemical process in the FTE it is known [31, 37] that with comparable values of electrical conductivity of the solid (CFM) and liquid (electrolyte), the distribution of the electrode potential along its thickness has a "parabolic" form (U-shaped curve), so that $E - E_{cp} > 0$, the value of $E - E_{cp}$ decreases in the interval $[0, x_{min}]$ and increases in the interval $[x_{min}, L]$, where x_{min} is the minimum point of the function $E(x)$. Consequently, the best distribution of potential, current density and metal deposit on the FTE with values of specific electrical conductivity and reaction surface distributed over the thickness of the electrode can be expected from the point of uniformity when the FTE consists of layers of CFM with the value of $\kappa(x)$ decreasing from 0 to the point x_{min} and increasing from x_{min} to L from layer to layer, and, conversely, the function $S_v(x)$ increasing from 0 to the point x_{min} and decreasing from x_{min} to L.

This conclusion is confirmed by calculations of the indicator of uniformity of potential distribution for the electrochemical system described above, when the best uniformity is observed when the distribution of specific electrical conductivity is in the form of a decreasing linear dependence, and the specific reaction surface is in the form of an increasing linear form, while the uniformity indicator is $\max E(x)/\min E(x) = 1.08$.

The specific distribution of the $S_v(x)$ function and the $\kappa(x)$ function is useful to consider when designing a FTE using carbon-graphite fiber materials with distributed specific electrical conductivity and specific reactive surface area as cathode materials.

Analysis of the Hamiltonian function allows us to identify a set of distributed parameters as the control function, including the related functions $\kappa(x)$, $S_v(x)$, κ_G.

$$u = u_2\,(1/u_1 + 1/\kappa_G). \qquad (16)$$

The selection of the control function in this form (16) may be useful when selecting the sequence of cathode blocks of a prefabricated FTE composed of various brands of CFM, taking into account the conclusions of the previous paragraph, that is, when u(x) decreases from the point $x = 0$ to the point $x = x_{min}$ and increases over the interval $[x_{min}, L]$. It should be noted that when considering the control function in the form (16), it may be necessary to take into account the distribution of the function $\kappa_G(x)$ – the specific electrical conductivity of the electrolyte solution.

The dependence of the electrical conductivity of the liquid phase of the system on the coordinate on the electrode is possible with a significant drop in the concentration of precipitating metal ions during the passage of the electrolyte through a three-dimensional flow electrode, as well as with intense gas formation, for example, during the electrochemical formation of hydrogen [16, 38]. Mathematical models, the development of which was carried out taking into account the influence of hydrogen release on the specific electrical conductivity of the liquid phase of an electrochemical system with a FTE, are published, for example, in [39]. In this paper, the modeling and calculation of such electrochemical systems is not considered.

RESULTS AND DISCUSSION

The mathematical models and methods for calculating and optimizing the galvanic coating of carbon fiber materials across the thickness of composite materials with cathodes made of carbon fiber composites (CFMs) with distributed values of specific electrical conductivity and specific reactive surface area discussed in this paper are aimed at correctly selecting the appropriate CFMs and their combination during the formation of composite materials to produce metallized CFMs with desired properties, in particular, with the best possible uniformity of metallic deposit distribution across the CFM thickness.

The mathematical models and methods for calculating the specific electrical conductivity and specific reactive surface area of carbon fiber composites presented in this paper enable dynamic simulation of electrochemical processes in FTEs, under non-stationary electrode conditions caused by changes in their properties during electrolysis.

The development of closed-loop mathematical models of electrochemical processes in FTEs with electrodes made of carbon fiber composites with distributed properties enabled the formulation of optimization problems for

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the galvanic metallization of carbon fiber composites in various forms, meeting specific criteria and technological requirements.

It is shown that during metallization of carbon fiber materials, the influence of distributed specific electrical conductivity and specific reaction surface are interrelated, which indicates the need for their joint consideration when solving problems of modeling and optimizing processes using FTEs made of CFMs.

In formulating the problem of optimizing the distribution of processes in the FTE through the correct selection of the electrical conductivity distributed across the electrode thickness and the reaction surface, the classical maximum method of L.S. Pontryagin was used, along with its simplified analogue based on natural simplifications and assumptions, as well as methods for directly calculating the best values of the desired distributed functions in the form of theoretically justified simplified forms.

CONCLUSION

The existing developed principles of the theory of metal electrodeposition on flow-through three-dimensional electrodes made of CFM, methods of mathematical modeling, and calculation of the distribution of electrochemical processes in the FTE enable the formulation and solution of problems of optimizing the process parameters of CFM metallization processes to create composite materials with specific properties.

Depending on the technological formulation of the problems of galvanic metallization of carbon-graphite materials, it is possible to select mathematical models and methods for solving problems in calculating the modes of electrodeposition and the design elements of flow-through three-dimensional cathodes made of CFM, and the existing variety of carbon-graphite material grades and modern methods of preliminary functionalization of the surface of carbon-graphite fibers by electrolysis in solutions of appropriate electrolytes make it possible to implement the found optimal conditions of electrochemical processes in solving specific problems of obtaining composite materials with specified technological parameters.

In this paper, the distributed specific electrical conductivity and specific reactive surface area of carbon fiber composites as electrode materials in flow-through three-dimensional electrodes are considered as control parameters for metal deposition processes in flow-through three-dimensional electrodes. Further development of mathematical models and optimization of processes in flow-through three-dimensional electrodes can be achieved by simulating and determining optimal transient galvanic and concentration modes of galvanic processes, as well as the methods and directions of electrolyte delivery and the overall current density within the flow-through three-dimensional electrode.

REFERENCES

1. Fialkov A.S. *Carbon. Interlayer composites and their basis*. Moscow: Aspect-Press;1997. (In Russ.).

2. Varentsov V.K., Belyakova Z.T. Effect of process parameters on the oxidation of cyanide-rhodanide ions on oxide anodes. *Non-ferrous metals*. 1984;2:95–97. (In Russ.).

3. Varentsov V.K., Varentsova V.I. Modification of electrode properties of carbon fibrous materials by electrolysis in aqueous solutions. *Electrochemistry*. 2001;37(7):811–820. (In Russ.).

4. Varentsov V.K., Varentsova V.I. Cadmium regeneration and changes in the properties of a carbon fiber electrode during electrolytic processing of ammonium cadmium plating wash solutions. *Journal of applied chemistry*. 2007;80(2):242–248. (In Russ.).

5. Varentsov V.K., Varentsova V.I., Bataev I.A., Serenko S.A. Synthesis of a carbon fiber material – manganese dioxide composite for ionistors by MnO_2 H_2O electrosorption. *Carbon: fundamental problems of science, materials science, technology. Structural and functional materials (including nanomaterials) and their production technologies*: 7th international conference. Vladimir: Vladimir state university publishing house, 2010:64–65. (In Russ.).

6. Varentsov V.K., Varentsova V.I. Electrolysis in electrolyte solutions – an effective method for modifying the properties of carbon fibrous materials. *Chemistry for sustainable development*. 2000;8(3):353–362. (In Russ.).

7. Varentsov V.K. *Electrochemical processes and equipment with volume-porous flow electrodes for extracting metals from dilute solutions*: dissertation for the degree of Doctor of Technical Sciences: specialty 05.17.03 "Technology of electrochemical processes and corrosion protection": defended on 14.02.90: approved on 06.07.90 / Varentsov Valery Konstantinovich. Sverdlovsk; 1990. (In Russ.).

8. Varentsov V.K., Koshev A.N., Varentsova V.I., Kuzina V.V. *Electrolyzers and electrochemical processes with flow-through three-dimensional carbon electrodes. Development fundamentals, mathematical modeling, theoretical and experimental research, industrial development*. Penza: Publishing house of Penza state university of architecture and contraction; 2025. ISBN 978-5-9282-1769-3 (In Russ.).

ISSN 2075-8545 (online)

9. Varentsov V.K., Koshev A.N. Mathematical modeling of electrochemical processes in flow-through three-dimensional electrodes. *Bulletin of the Siberian Branch of the USSR Academy of Sciences. Chemical Sciences Series*. 1988;17:117–125. (In Russ.).

10. Varentsov V.K., Koshev A.N., Sukhov I.F., Kuzina V.V. *Theoretical foundations and modeling of electrochemical processes in systems with flow-through three-dimensional electrodes*. Penza: Publishing house of Penza state university of architecture and contraction; 2014. ISBN 978-5-9282-1152-3 (In Russ.).

11. Varentsov V.K., Koshev A.N., Varentsova V.I., Kuzina V.V. *Oxidation-reduction processes on flow-through three-dimensional electrodes. Mathematical modeling, theory, experiment*. Penza: Publishing house of Penza state university of architecture and contraction; 2020. ISBN 978-5-9282-1660-3 (In Russ.).

12. Koshev A.N., Glazer G.N., Varentsov V.K. Mathematical model of the electrolysis process on a flow-through volume-porous electrode with variable electrical conductivity of the system. *Electrochemistry*. 1992;28(8):1270–1274. (In Russ.).

13. Koshev A.N., Varentsov V.K., Chirkina M.A., Kamburg V.G. Mathematical modeling and theory of polarization distribution in electrochemical reactors with flow-through volume-porous cathodes. *Mathematical modeling*. 2011;23(8):110–126. (In Russ.).

14. Koshev A.N., Varentsov V.K., Kamburg V.G. Mathematical modeling of the process of electrodeposition of metals from multicomponent systems on flow-through volumetric-porous electrodes. *Bulletin of the Siberian Branch of the USSR Academy of Sciences. Series of Chemical Sciences*. 1984;6:24–27.

15. Koshev A.N., Kuzina V.V. Modeling and calculation of the concentration of the electroactive component in the electrolysis process. *Control of large systems*. 2011;33:233–252. (In Russ.).

16. Koshev A.N., Glazer G.N., Varentsov V.K. On the effect of gas formation in the pores of a flow-through volume-porous cathode on the electrical conductivity of the electrolyte. *Electrochemistry*. 1992;28(8):1160–1170. (In Russ.).

17. Koshev A.N., Varentsov V.K., Sukhov I.F., Gvozdeva I.G. Processes in a porous electrode in the case of distributed electrolyte flow velocity. *Mathematical modeling*. 2013;24(2):87–101. (In Russ.).

18. Kuzina V.V., Samchenko S.V., Kozlova I.V., Koshev A.N. Mathematical modeling of physical and chemical processes in porous media in solving the problems of nanocomposite materials and water-filling. *Nanotechnologies in construction*. 2023;15(4):298–309. https://doi.org/10.15828/2075-8545-2023-15-4-298-309. – EDN: HJIEDH.

19. Koshev A.N., Kuzina V.V. Distributed reaction surface of carbon-graphite volume-porous cathodes as a parameter for optimizing of metallization process of composite and nanocomposite materials. *Nanotechnologies in Construction*. 2025;17(2):119–131. https://doi.org/10.15828/2075-8545-2025-17-2-119-131. – EDN: XWDYCA.

20. Newman J.S., Tiedemann W. Flow-through porous electrodes. *Adv. Electrochem. and Electrochemical Eng*. 1978;11:353–458.

21. Koshev A.N., Chirkina M.A., Varentsov V.K. Nonstationary mathematical models of the electrochemical processes in volumetric porous flow electrodes. *Russ. J. Electrochem*. 2007;43(11):1299–1304.

22. Koshev A.N., Gvozdeva I.G., Koshev N.A., Varentsov V.K. Calculation of the optimal electrical conductivity of flow-through volumetric-porous cathodes. *Control of large systems*. 2012;37:232–249. (In Russ.).

23. Koshev A.N., Varentsov V.K., Sukhov I.F. Calculation of effective conductivity profile of electrochemical reactor with flow-type three-dimensional electrodes. *Theoretical foundations of chemical technology*. 2014;48(2):180–187.

24. Varentsov V.K., Koshev A.N., Varentsova V.I., Kuzina V.V. *Carbon fiber electrodes: properties, modification, processes, and electrolyzers. Mathematical modeling and optimization*. Penza: Publishing house of Penza state university of architecture and contraction; 2021. (In Russ.).

25. Varentsov V.K., Zherebilov A.F., Maley M.D. Carbon-graphite fiber materials: new electrodes for extracting metals from dilute solutions. 1. Non-woven materials. *Bulletin of the Siberian Branch of the USSR Academy of Sciences. Series of chemical sciences*. 1984;17(6):120–127 (In Russ.).

26. Varentsov V.K. Potential and prospects of electrolysis in hydrometallurgy of gold and silver. *Chemistry, technology, and analysis of gold and silver*: Abstracts of reports of the 1st All-Union Conference. Novosibirsk; 1983. (In Russ.).

27. Konkin A.A. *Carbon and other heat-resistant fibrous materials*. Moscow: Chemistry; 1974. (In Russ.).

28. Ermolenko I.N., Lyubliner I.P., Gulko N.V. *Element-containing carbon fibrous materials*. Minsk: Science and Technology; 1982. (In Russ.).

29. Koshev A.N., Varentsov V.K., Glazer G.N. On the issue of determining the electrolysis-accessible surface of a porous electrode. *Electrochemistry*. 1992;28(9):1404. (In Russ.).

30. Koshev A.N., Varentsov V.K., Chirkina M.A. Analysis of mathematical models and theory of polarization distribution of flow-through bulk-porous electrodes. *Physical chemistry of surfaces and protection of materials*. 2009;45(4):441–448. (In Russ.).

ISSN 2075-8545 (online)

31. Varentsov V.K., Koshev A.N., Varentsova V.I., Kuzina V.V. *Redox processes on flow-through three-dimensional electrodes. Mathematical modeling. Theory. Experiment*. Penza: Publishing house of Penza state university of architecture and contraction, 2020. (In Russ.).

32. Gvozdeva I.G., Koshev A.N., Varentsov V.K., Kuzina V.V. Stability and solvability problems in mathematical modeling of electrochemical process distribution in a flow-through three-dimensional electrode. *XXI Century: results of the past and problems of the present*. 2021;V.10;4(56):39–43. (In Russ.).

33. Koshev A.N., Varentsov V.K. Boundary conditions for differential equations describing electrochemical processes in reactors with three-dimensional flow electrodes. *Mathematical modeling*. 2014:26(2):11–23. (In Russ.).

34. Gvozdeva I.G., Koshev A.N. Computer program registration certificate RU 2025695790, 12/15/2025. Application No. 2025694325 dated 12/04/2025.

ADDITIONAL INFORMATION

The authors declare that generative artificial intelligence technologies and technologies based on artificial intelligence were not used in the preparation of the article.

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Alexander N. Koshev – scientific supervision, formulation of the task of mathematical modeling, development of modeling methodology, development of computer programs, text writing, final conclusions.

Valentina V. Kuzina – mathematical modeling, development of computer programs, carrying out calculations, revision of the text.

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