Mathematical modeling of diffusion transfer for charged particles in the layered composite medium

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Abstract

Using the methods of the integral Laplace transform and fundamental Cauchy functions, for the first time, an exact analytical solution of the mathematical model of the adsorption mass transfer of charged particles for an inhomogeneous cylindrical limited composite medium with a symmetrical cavity and a system of *n* interface boundaries with specified 2*n*+2 non-stationary mass transfer modes was constructed for the first time. New recurrent algorithms and computational procedures have been developed for constructing influence functions generated by system inhomogeneities, boundary conditions, and a system of interface conditions.

Keywords 1

Micro- and nanoporous systems, inhomogeneous cylindrical media, mass transfer, inhomogeneous boundary conditions, interface conditions, Laplace transformations, fundamental functions.

1. Introduction

The development of modern nanotechnologies and the aging of the latest nanostructures and materials pose new challenges for studying the mechanisms of kinetics and intensification of diffusion-adsorption mass transfer in heterogeneous multilayer medias of various configurations. The study of the processes of adsorption mass transfer in inhomogeneous media with a cellular structure today requires the development of new qualitative modeling methods that make it possible to describe the complex mechanisms of the system of interface interactions between all components of the transfer and unsteady modes of mass transfer on mass transfer surfaces. Problems of mathematical modeling of diffusion-adsorption mass transfer in homogeneous and inhomogeneous porous media and methods for constructing mathematical solutions of such models were considered in papers [1-3]. For homogeneous media of adsorption mass transfer, the methods of integral transformations of Fourier, Laplace, Weber, Hankel and Hilbert were used. For inhomogeneous media, numerous methods were mainly used [4-6]. Mathematical theory of integral transformations and their applications for mass transfer problems for inhomogeneous and porous media, taking into account the system of mechanisms of interface interactions between transfer elements and non-stationary modes of mass transfer on mass transfer surfaces (taking into account the spectral parameter in the boundary conditions and the system of interface conditions (conjugation)]. assumptions on the structures of differential operators Fourier, Bessel, Weber, Hankel, boundary conditions and interface conditions, integral Fourier, Bessel, Weber and Hankel transforms with a spectral parameter for inhomogeneous *n*+1-complex bounded, semi-bounded and unbounded are constructed and the main solutions of transport models are constructed (fundamental Cauchy and Green functions) are the functions of the influence of the inhomogeneities of the problem, the boundary conditions and the system of interface

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conditions. In paper [2] we considered a mathematical model of adsorption mass transfer in an inhomogeneous limited n-interface nanoporous medium, the exact analytical solution of the model is constructed and the components of the influence matrices of (principal) solutions of the system are written out.

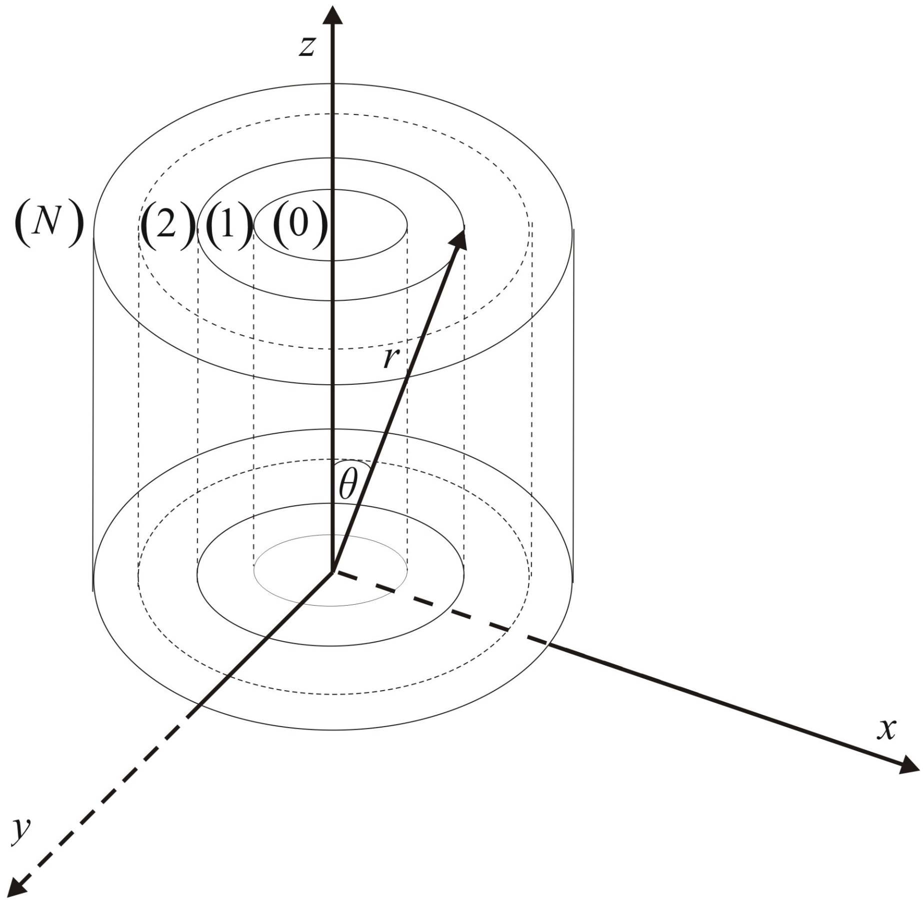

Figure 1: Geometric scheme of a layered microstructure with marked coordinates of the boundaries of the separation of media

2. Mathematical description of the problem

Adsorption mass transfer in an inhomogeneous limited cylindrical n-interface adsorption medium in coordinate r filled with n adsorbents with different physicochemical characteristics is considered. The geometric scheme of the studied layered microstructure is as shown in Fig.1. The mathematical model of such a transfer, taking into account the non-stationarity of mass transfer on mass transfer surfaces (edge surfaces and contact surfaces $r = R_{j-1}, j = \overline{1,n}$) and the physical assumptions given in [2-4], can be described in the form of such a mixed boundary value problem: to construct limited in the region $D_n = \left\{ (t,r) : t > 0, r \in \bigcup_{j=1}^{n+1} (R_{j-1}, R_j), R_0 > 0, R_{n+1} \le \infty \right\}$ a solution of the system of partial differential equations:

$$\frac{\partial C_j(t,r)}{\partial t} + \frac{\partial a_j(t,r)}{\partial t} + \eta_j^2 C_j = D_{r_j} B_{\nu\alpha_j} \left[C_j \right] + f_j(t,r); \qquad (1)$$

$$\frac{\partial a_j}{\partial t} = \beta_j (C_j - \gamma_j a_j); \qquad (2)$$

with following initial conditions:

$$C_j(t,r)_{t=0} = C_{0_j}(r); a_j(t,r)_{t=0} = a_{0_j}(r); \qquad (3)$$

and such boundary conditions and a system of interface (conjugation) conditions along the geometric coordinate r:

$$[(\alpha_{12}^0+\delta_{12}^0\frac{\partial}{\partial t})\frac{\partial}{\partial r}+(\beta_{12}^0+\gamma_{12}^0\frac{\partial}{\partial t})]C_1(t,r)\big|_{r=R_0}=\omega_1(t);$$

$$[(\alpha_{22}^{n+1}+\delta_{22}^{n+1}\frac{\partial}{\partial t})\frac{\partial}{\partial r}+(\beta_{22}^{n+1}+\gamma_{22}^{n+1}\frac{\partial}{\partial t})]C_{n+1}(t,r)\big|_{r=R_{n+1}}=\omega_{n+1}(t) \qquad (4)$$

$$\left[[(\alpha_{i1}^j+\delta_{i1}^j\frac{\partial}{\partial t})\frac{\partial}{\partial r}+(\beta_{i1}^j+\gamma_{i1}^j\frac{\partial}{\partial t})]C_j(t,r)-[(\alpha_{i2}^j+\delta_{i2}^j\frac{\partial}{\partial t})\frac{\partial}{\partial r}+(\beta_{i2}^j+\gamma_{i2}^j\frac{\partial}{\partial t})]C_{j+1}(t,r)\right]\Bigg|_{r=R_j}=0; \qquad (5)$$

$$j=\overline{1,n};i=\overline{1,2}$$

Here $B_{\nu\alpha_j}=\frac{d^2}{dr^2}+\frac{1}{r}(2\alpha_j+1)\frac{d}{dr}-(\nu_j^2-\alpha_j^2)r^{-2}$ is the Bessel operator for n-interface environment, C_j,a_j - mass concentrations of the adsorbent, respectively, in the liquid phase (interparticle space) and the solid phase (in micro- and nanopores of adsorbent grains) for the jth layer of the adsorption medium, $j=\overline{1,n+1}$.

2.1. Methodology for constructing the analytical solution of the model and recurrent algorithms for calculating the matrices of the impact functions (main solutions)

Assuming that the desired vector functions $C(t,r),a(t,r)$ are Laplace originals, we apply the Laplace integral transformation with respect to the time variable t to the boundary value problem (1)-(5). As a result, we obtain a boundary value problem: to construct a solution of the system of Bessel differential equations bounded on the set $I_n=\left\{r:r\in\bigcup_{j=1}^{n+1}(R_{j-1},R_j),R_0>0,R_{n+1}<\infty\right\}$ for the modified functions:

$$\left[B_{\nu\alpha_j}-q_j^2(p)\right]C_j^*(p,r)=-\mathcal{F}_j^*(p,r) \qquad (6)$$

by boundary conditions

$$[\bar{\alpha}_{12}^0\frac{\partial}{\partial r}+\bar{\beta}_{12}^0]C_1^*(p,r)\big|_{r=R_0}=\omega_{R_0}^*(p);\ [\bar{\alpha}_{22}^{n+1}\frac{\partial}{\partial r}+\bar{\beta}_{22}^{n+1}]C_{n+1}^*(p,r)\big|_{r=R_{n+1}}=\omega_{R_{n+1}}^*(p) \qquad (7)$$

and interface conditions along the coordinate r:

$$\left[[(\bar{\alpha}_{i1}^j\frac{d}{dz}+\bar{\beta}_{i1}^j\frac{d}{dt})]C_j^*(p,z)-(\bar{\alpha}_{i2}^k\frac{d}{dz}+\bar{\beta}_{i2}^k\frac{d}{dt})]C_{j+1}^*(p,r)\right]\Bigg|_{r=R_j}=\omega_{ij};j=\overline{1,n};i=\overline{1,2}. \qquad (8)$$

Here

$$\mathcal{F}_j^*(p,r)=\frac{1}{D_{r_j}}[f_j^*(p,r)+C_{o_j}(r)+\frac{\beta_j\gamma_j}{p+\beta_j\gamma_j}a_{0_j}(r)]. \qquad (9)$$

$$\omega_{R_0}^*(p)=\omega_1^*(p)+\left(\delta_{12}^0\frac{d}{dr}+\gamma_{12}^0\right)C_{0_1}(R_0)\equiv\omega_1^*(p)+\omega_{1,1};$$

$$\omega_{R_{n+1}}^*(p)=\omega_{n+1}^*(p)+\left(\delta_{22}^{n+1}\frac{d}{dr}+\gamma_{22}^{n+1}\right)C_{0_{n+1}}(R_{n+1})\equiv\omega_{n+1}^*(p)+\omega_{n+1,1};. \qquad (10)$$

$$\omega_{ij}=\left[\left(\delta_{i1}^j\frac{d}{dr}+\gamma_{i1}^j\right)C_{0_i}(r)-\left(\delta_{i2}^j\frac{d}{dr}+\gamma_{i2}^j\right)C_{0_{j+1}}(r)\right]\Bigg|_{r=R_j}; \qquad (11)$$

$$q_j^2(p)=\frac{1}{D_{r_j}\left(p+\beta_j\gamma_j\right)}\left[p^2+p\left(\beta_j(1+\gamma_j)+\beta_j\gamma_j\cdot\eta_j^2\right)\right]$$

$$\bar{\alpha}_{im}^j=\alpha_{im}^j+\delta_{im}^j\cdot p;\bar{\beta}_{im}^j=\beta_{im}^j+\gamma_{im}^j\cdot p;j=\overline{1,n};i,m=\overline{1,2}. \qquad (12)$$

Wherein we have

$$a_j^*(p,r) = \frac{a_{0j}(r)}{p+\beta_j\gamma_j} + \frac{\beta_j(r)}{p+\beta_j\gamma_j} C_j^*(p,r);\ j=\overline{1,n+1}. \quad (13)$$

If we fix a branch of the two-sheeted function, on which $\operatorname{Re} q_j(p) > 0$, due to the properties of the functions that form the fundamental system of solutions of the Bessel equation (6), we construct the solution of the inhomogeneous boundary value problem (6)-(8) by the method of Cauchy functions [3]:

$$C_j^*(p,r) = A_j \cdot I_{\nu\alpha_j}(q_j r) + B_j \cdot K_{\nu\alpha_j}(q_j r) + \int_{R_{j-1}}^{R_j} \mathcal{E}_{\nu\alpha_j}^*(p,r,\rho)\mathcal{F}_j^*(p,\rho)\rho^{2\alpha_j+1}d\rho,\ j=\overline{1,n+1}. \quad (14)$$

where $\mathcal{E}_{\nu\alpha_j}^*(p,r,\rho),\ j=\overline{1,n+1}$ is the Cauchy which satisfy following conditions:

$$\begin{cases} \mathcal{E}_{\nu\alpha_j}^*(p,r,\rho)\Big|_{r=\rho+0} - \mathcal{E}_{\nu\alpha_j}^*(p,r,\rho)\Big|_{r=\rho-0} = 0; \\ \dfrac{d}{dr}\mathcal{E}_{\nu\alpha_j}^*(p,r,\rho)\Big|_{r=\rho+0} - \dfrac{d}{dr}\mathcal{E}_{\nu\alpha_j}^*(p,r,\rho)\Big|_{r=\rho-0} = -\rho^{-(2\alpha_j+1)}. \end{cases} \quad (15)$$

The Cauchy functions $\mathcal{E}_{\nu\alpha_j}^*(p,r,\rho),\ j=\overline{1,n+1}$ are found in the following form:

$$\mathcal{E}_{\nu\alpha_j}^*(p,r,\rho) = \begin{cases} \mathcal{E}_{\nu\alpha_j}^{-*} = D_{1_j} I_{\nu_j\alpha_j}(q_j r) + E_{1_j} K_{\nu_j\alpha_j}(q_j r);\ R_{j-1} < r < \rho < R_j \\ \mathcal{E}_{\nu\alpha_j}^{+*} = D_{2_j} I_{\nu_j\alpha_j}(q_j r) + E_{2_j} K_{\nu_j\alpha_j}(q_j r);\ R_{j-1} < \rho < r < R_j \end{cases}. \quad (16)$$

at the same time, they must satisfy additional homogeneous conditions for the left and right interfaces

$$\left(\bar{\alpha}_{12}^{j-1}\frac{d}{dr} + \bar{\beta}_{12}^{j-1}\right)\mathcal{E}_{\nu\alpha_j}^{-*}\Big|_{r=R_{j-1}} = 0, \quad (17)$$

$$\left(\bar{\alpha}_{11}^{j}\frac{d}{dr} + \bar{\beta}_{11}^{j}\right)\mathcal{E}_{\nu\alpha_j}^{+*}\Big|_{r=l_j} = 0, \quad (18)$$

Let us consider the following functions:

$$U_{\nu\alpha_{im}}^{j1}(q_s R_j) = (\bar{\alpha}_{im}^j \frac{d}{dz} + \bar{\beta}_{im}^j) I_{\nu_j\alpha_j}(q_s r)\Big|_{r=R_j} = (\bar{\alpha}_{im}^j \frac{\nu_j-\alpha_j}{R_j} + \bar{\beta}_{im}^j) I_{\nu_j\alpha_j}(q_s R_j) + \bar{\alpha}_{im}^j R_j q_s^2 I_{\nu_j+1,\alpha_j+1}(q_s R_j);$$
$$U_{\nu\alpha_{im}}^{j2}(q_s R_j) = (\bar{\alpha}_{im}^j \frac{d}{dr} + \bar{\beta}_{im}^j) K_{\nu_j\alpha_j}(q_s r)\Big|_{r=R_j} = (\bar{\alpha}_{im}^j \frac{\nu_j-\alpha_j}{R_j} + \bar{\beta}_{im}^j) K_{\nu_j\alpha_j}(q_s R_j) - \bar{\alpha}_{im}^j R_j q_s^2 K_{\nu_j+1,\alpha_j+1}(q_s R_j) \quad (19)$$

$$\Phi_{\nu\alpha_{im}}^j(q_s R_j, q_s r) = U_{\nu\alpha_{im}}^{j1}(q_s R_j)\cdot K_{\nu_j\alpha_j}(q_s r) - U_{\nu\alpha_{im}}^{j2}(q_s R_j)\cdot I_{\nu_j\alpha_j}(q_s r). \quad (20)$$

To determine the constants $D_{1_k}, E_{1_k}, D_{2_k}, E_{2_k}$ and Cauchy functions $\mathcal{E}_k^*(p,r,\rho), k=\overline{1,n}$ as a result of their properties determined by conditions (19), (20), we obtain the algebraic system of equations:

$$(D_{2_k} - D_{1_k}) I_{\nu_k\alpha_k}(q_k\rho) + (E_{2_k} - E_{1_k}) K_{\nu_k\alpha_k}(q_k\rho) = 0;$$
$$(D_{2_k} - D_{1_k})\left(\frac{\nu_k-\alpha_k}{\rho} I_{\nu_k\alpha_k}(q_k\rho) + R_k q_k^2 I_{\nu_k+1,\alpha_k+1}(q_k\rho)\right) +$$
$$+(E_{2_k} - E_{1_k})\left(\frac{\nu_k-\alpha_k}{\rho} K_{\nu_k\alpha_k}(q_k\rho) - R_k q_k^2 K_{\nu_k+1,\alpha_k+1}(q_k\rho)\right) = -\frac{1}{q_k\cdot\rho^{2\alpha_k+1}}; \quad (21)$$
$$D_{1_k}\cdot U_{\nu\alpha_{12}}^{k-1,1}(q_k R_{k-1}) + E_{1_k}\cdot U_{\nu\alpha_{12}}^{k-1,2}(q_k R_{k-1}) = 0;$$
$$D_{2_k}\cdot U_{\nu\alpha_{11}}^{k1}(q_k R_k) + E_{2_k}\cdot U_{\nu\alpha_{11}}^{k,2}(q_k R_k) = 0.$$

From the algebraic system of equations (21) we find:

$$D_{2_k} - D_{1_k} = -q_k^{2\alpha_k} K_{\nu_k\alpha_k}(q_k\rho),\ E_{2_k} - E_{1_k} = q_k^{2\alpha_k} I_{\nu_k\alpha_k}(q_k\rho). \quad (22)$$

As a result of the single-valued openness of the algebraic system (21), the Cauchy functions $\mathcal{E}^*_k(p,r,\rho); k=\overline{1,n+1}$ are defined and, as a result of symmetry with respect to the diagonal $r=\rho$, have the following structure:

$$\mathcal{E}^*_{\nu\alpha_k}(p,r,\rho)=\frac{q_k^{2\alpha_k}}{\Delta_{\alpha_{11}}\left(q_kR_{k-1},q_kR_k\right)}\begin{cases}\Phi^k_{\nu\alpha_{11}}\left(q_kR_k,q_k\rho\right)\cdot\Phi^{k-1}_{\nu\alpha_{12}}\left(q_kR_{k-1},q_kr\right), R_{k-1}<r<\rho<R_k\\ \Phi^k_{\nu\alpha_{11}}\left(q_kR_k,q_kr\right)\cdot\Phi^{k-1}_{\nu\alpha_{12}}\left(q_kR_{k-1},q_k\rho\right), R_{k-1}<\rho<r<R_k\end{cases}. \tag{23}$$

where

$$\begin{gathered}\Delta_{\nu\alpha_{im}}(q_kR_{k-1},q_kR_k)=U^{k-1,1}_{\nu\alpha_{k_i2}}(q_kR_{k-1})U^{k,2}_{\nu\alpha_{k_m1}}(q_kR_k)-U^{k-1,2}_{\nu\alpha_{k_i2}}(q_kR_{k-1})U^{k,1}_{\nu\alpha_{k_m1}}(q_kR_k)\\ k=\overline{2,n}; i,m=\overline{1,2}\\ \Delta_{\nu\alpha_{11}}(q_{n+1}R_n,q_{n+1}R_{n+1})=U^{n,1}_{\nu\alpha_{n+1_i2}}(q_{n+1}R_n)U^{n+1,2}_{\nu\alpha_{n+1_{22}}}(q_{n+1}R_{n+1})-U^{n,2}_{\nu\alpha_{n+1_i2}}(q_{n+1}R_n)U^{n+1,1}_{\nu\alpha_{n+1_{22}}}(q_{n+1}R_{n+1});\\ i=\overline{1,2}.\end{gathered} \tag{24}$$

With known Cauchy functions $\mathcal{E}^*_{\nu\alpha_j}(p,r,\rho)$, the boundary conditions at the points $r=R_0$ and $r=R_{n+1}$ the interface conditions (7) for determining the unknown coefficients $A_j, B_j, j=\overline{1,n+2}$ participating in the structures (14) of the general solution of the boundary value problem (6)-(8) $C^*_j(p,r)$ give an algebraic system with $2n+2$ equations:

$$\begin{cases}U^{n,1}_{\nu\alpha_{11}}\left(q_nR_n\right)\left(q_nl_n\right)A_n+U^{n,2}_{\nu\alpha_{11}}\left(q_nR_n\right)B_n-U^{n,1}_{\nu\alpha_{12}}\left(q_{n+1}R_n\right)A_{n+1}-U^{n,2}_{\nu\alpha_{12}}\left(q_{n+1}R_n\right)B_{n+1}=\omega_{1_n}\\ U^{n,1}_{\nu\alpha_{21}}\left(q_nR_n\right)A_n+U^{n,2}_{\nu\alpha_{21}}\left(q_nR_n\right)B_n-U^{n,1}_{\nu\alpha_{22}}\left(q_{n+1}R_n\right)A_{n+1}-U^{n,2}_{\nu\alpha_{22}}\left(q_{n+1}R_n\right)B_{n+1}=\omega_{2_n}+G^*_n\\ U^{n+1,1}_{\nu\alpha_{22}}\left(q_{n+1}R_{n+1}\right)A_{n+1}+U^{n+1,2}_{\nu\alpha_{22}}\left(q_{n+1}R_{n+1}\right)B_{n+1}=\omega^*_{R_{n+1}}\left(p\right)\end{cases} \tag{25}$$

Here, the expressions containing the integrals of the Cauchy functions $\mathcal{E}^*_{\nu\alpha_j}(p,r,\rho)$ in (25) and are calculated by the formula:

$$G^*_j=\frac{c_{1_j}}{R_j^{2\alpha_j+1}}\int_{R_{j-1}}^{R_j}\frac{\Phi^{j-1}_{\nu\alpha_{12}}(q_jR_{j-1},q_j\rho)}{\Delta_{\nu\alpha_{11}}(q_jR_{j-1},q_jR_{j-1})}\mathcal{F}^*_j(p,\rho)\rho^{2\alpha_j+1}d\rho-\frac{c_{2_j}}{R_j^{2\alpha_{j+1}+1}}\int_{R_j}^{R_{j+1}}\frac{\Phi^{j+1}_{\nu\alpha_{11}}(q_{j+1}R_{j+1},q_{j+1}\rho)}{\Delta_{\nu\alpha_{11}}(q_{j+1}R_j,q_{j+1}R_{j+1})}\mathcal{F}^*_{j+1}(p,\rho)\rho^{2\alpha_{j+1}+1}d\rho. \tag{26}$$

Next we suppose that the fulfilled condition for the unique solvability of the boundary value problem (6)-(8), that is, the determinant of the algebraic system (25) is non-zero:

$$\Delta^*_{\nu\alpha}(p)\equiv\det A_{\nu\alpha}(p)\neq 0\,. \tag{27}$$

As a result of the unique solvability of the algebraic system (25) and the substitution of the obtained values $A_k, B_k, D_{1_k}, D_{2_k} E_{1_k}, E_{2_k}, k=\overline{1,n+1}$ into (14), the components of the solution of the boundary value problem (6)-(8) is can be obtained. After a series of transformations (expanding the determinants $\Delta^*_{A_k}I_{\nu_k\alpha_k}(q_kr)+\Delta^*_{B_k}K_{\nu_k\alpha_k}(q_kr), k=\overline{1,n+1}$) we obtain recursive expressions for calculating the components $C^*_k(p,r)$ of the vector function $C^*(p,r)$ - the solution of the boundary value problem (6)-(8) in the form:

$$\begin{gathered}C^*_k(p,r)=W^*_{k_1}(p,r)\cdot\omega^*_{R_0}(p)+W^*_{k_{n+1}}(p,r)\cdot\omega^*_{R_{n+1}}(p)+\sum_{j=1}^{n}\left[\mathcal{R}^*_{1_{k,j}}(p,r)\cdot\omega_{1_j}+\mathcal{R}^*_{2_{k,j}}(p,r)\cdot\omega_{2_j}\right]+\\ +\sum_{j=1}^{n+1}\int_{R_{j-1}}^{R_j}\mathcal{H}^*_{\nu\alpha_{k,j}}(p,r,\rho)\cdot\mathcal{F}^*_j(p,\rho)\rho^{2\alpha_j+1}d\rho; k=\overline{1,n+1}.\end{gathered} \tag{28}$$

Here the main solutions of the boundary value problem (6)-(8) have are obtained as follows.

Functions of the influence of the left boundary condition $\omega^*_{R_0}(p)$ on the kth segment of the adsorption medium $W^*_{k_1}(p,r)$:

$$W_{k_1}^*(p,r)=\begin{cases}\dfrac{1}{\Delta_{\nu\alpha}^*(p)}\left[\Phi_{\nu\alpha_{21}}^1(q_1R_1,q_1r)\Delta'_{\overline{1,2}}-\Phi_{\nu\alpha_{11}}^1(q_1R_1,q_1r)\Delta_{\overline{1,2}}\right] & ;k=1\\ \dfrac{1}{\Delta_{\nu\alpha}^*(p)}\prod_{s=1}^{k-1}\dfrac{-c_{1_s}}{q_s^{2\alpha_s}R_s^{2\alpha_s+1}}\left[\Phi_{\nu\alpha_{21}}^{k-1}(q_kR_k,q_kr)\cdot\Delta'_{\overline{1,2k}}-\Phi_{\nu\alpha_{11}}^{k}(q_kR_k,q_kr)\cdot\Delta_{\overline{1,2k}}\right] & ;k=\overline{1,n}\\ -\dfrac{1}{\Delta_{\nu\alpha}^*(p)}\prod_{s=1}^{n}\dfrac{-c_{1_s}}{q_s^{2\alpha_s}R_s^{2\alpha_s+1}}\Phi_{\nu\alpha_{11}}^{n+1}(q_{n+1}r,q_{n+1}R_{n+1})\cdot & k=n+1\end{cases}\tag{29}$$

Functions of the impact of the right boundary condition on the kth segment of the adsorption medium $W_{n+1_k}^*(p,r)$:

$$W_{k_{n+1}}^*(p,z)=\begin{cases}-\dfrac{1}{\Delta_{\nu\alpha}^*(p)}\prod_{s=1}^{n}\dfrac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}\Phi_{\nu\alpha_{12}}^0(q_1R_0,q_1r) & ;k=1\\ -\dfrac{1}{\Delta_{\nu\alpha}^*(p)}\prod_{s=k}^{n}\dfrac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}\left[\Phi_{\nu\alpha_{22}}^{k-1}(q_kR_{k-1},q_kr)\cdot\Delta_{\overline{1,2k-2}}-\Phi_{\nu\alpha_{12}}^{k-1}(q_kR_{k-1},q_kr)\cdot\Delta'_{\overline{1,2k-2}}\right] & ;k=\overline{1,n}\\ \dfrac{1}{\Delta_{\nu\alpha}^*(p)}\left[\Phi_{\nu\alpha_{12}}^n(q_{n+1}r,q_{n+1}R_n)\cdot\Delta'_{\overline{1,2n}}-\Phi_{22}^n(q_{n+1}r,q_{n+1}R_n)\cdot\Delta_{\overline{1,2n}}\right] & ;k=n+1\end{cases}\tag{30}$$

Functions of the influence of the jth source on the kth segment of the adsorption medium are obtained as follows:

$$\mathcal{H}_{\nu\alpha_{11}}^*(p,r,\rho)=\frac{q_1^{2\alpha_1}}{\Delta_{\nu\alpha}^*(p)}\begin{cases}\Phi_{\nu\alpha_{12}}^0(q_1R_0,q_1\rho)\cdot\left[\Phi_{\nu\alpha_{11}}^1(q_1r,q_1R_1,)\mathrm{A}_{\overline{1,2}}-\Phi_{\nu\alpha_{21}}^1(q_1r,q_1R_1)\mathrm{A}'_{\overline{1,2}}\right],R_0<\rho<r<R_1\\ \Phi_{\nu\alpha_{12}}^0(q_1R_0,q_1r)\cdot\left[\Phi_{\nu\alpha_{11}}^1(q_1\rho,q_1R_1,)\mathrm{A}_{\overline{1,2}}-\Phi_{\nu\alpha_{21}}^1(q_1\rho,q_1R_1)\mathrm{A}'_{\overline{1,2}}\right],R_0<r<\rho<R_1\end{cases}\tag{31}$$

$j=\overline{2,n}$

$$\mathcal{H}_{\nu\alpha_{1_j}}^*(p,r,\rho)=\frac{q_j^{2\alpha_j}\cdot\prod_{s=1}^{j-1}\dfrac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}}{\Delta_{\nu\alpha}^*(p)}\Phi_{\nu\alpha_{12}}^0(q_1R_0,q_1r)\left[\Phi_{\nu\alpha_{11}}^j(q_jR_j,q_j\rho)\mathrm{A}_{\overline{1,2j}}-\Phi_{\nu\alpha_{21}}^j(q_jR_j,q_j\rho)\mathrm{A}'_{\overline{1,2j}}\right]\tag{32}$$

$j=\overline{2,n}$

$$\mathcal{H}_{\nu\alpha_{1,n+1}}^*(p,r,\rho)=\frac{q_{n+1}^{2\alpha_{n+1}}\prod_{s=1}^{n}\dfrac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}}{\Delta_{\nu\alpha}^*(p)}\cdot\Phi_{\nu\alpha_{12}}^0(q_1R_0,q_1r)\Phi_{\nu\alpha_{11}}^{n+1}(q_{n+1}\rho,q_{n+1}R_{n+1})\tag{33}$$

impact of the j -th source ($j=\overline{2,k-1}$) on the kth segment ($k=\overline{2,n}$) of the adsorption medium:

$$\mathcal{H}_{\nu\alpha_{kj}}^*(p,r,\rho)=-\frac{q_j^{2\alpha_j}\prod_{s=j}^{k-1}\dfrac{-c_{1_s}}{q_s^{2\alpha_s}R_s^{2\alpha_s+1}}}{\Delta_{\nu\alpha}^*(p)}\left[\Phi_{\nu\alpha_{21}}^k(q_kR_k,q_kr)\mathrm{A}'_{\overline{1,2k}}-\Phi_{\nu\alpha_{11}}^k(q_kR_k,q_kr)\mathrm{A}_{\overline{1,2k}}\right]\cdot$$
$$\cdot\left[\Phi_{\nu\alpha_{22}}^{j-1}(q_jR_{j-1},q_j\rho)\cdot\Delta_{\overline{1,2j-2}}-\Phi_{\nu\alpha_{12}}^{j-1}(q_jR_{j-1},q_j\rho)\cdot\Delta'_{\overline{1,2j-2}}\right];j=\overline{2,k-1};k=\overline{2,n}\tag{34}$$

Then, in the general case, for the action functions it turns out:

$$\mathcal{H}_{\nu\alpha_{kk}}^*(p,r,\rho)=\frac{q_k^{2\alpha_k}}{\Delta_{\nu\alpha}^*(p)}\begin{cases}[\Phi_{\nu\alpha_{22}}^{k-1}(q_kR_{k-1},q_k\rho)\cdot\Delta_{\overline{1,2k-2}}-\Phi_{\nu\alpha_{12}}^{k-1}(q_kR_{k-1},q_k\rho)\cdot\Delta'_{\overline{1,2k-2}}]\cdot\\ [\Phi_{\nu\alpha_{22}}^{k-1}(q_kR_{k-1},q_kr)\cdot\Delta_{\overline{1,2k-2}}-\Phi_{\nu\alpha_{12}}^{k-1}(q_kR_{k-1},q_kr)\cdot\Delta'_{\overline{1,2k-2}}]\cdot\end{cases}$$
$$\cdot[\Phi_{\nu\alpha_{21}}^k(q_kR_k,q_kr)\cdot\mathrm{A}'_{\overline{1,2k}}-\Phi_{\nu\alpha_{11}}^k(q_kR_k,q_kr)\cdot\mathrm{A}_{\overline{1,2k}}],R_{k-1}<\rho<r<R_k$$
$$\cdot[\Phi_{\nu\alpha_{21}}^k(q_kR_k,q_k\rho)\cdot\mathrm{A}'_{\overline{1,2k}}-\Phi_{\nu\alpha_{11}}^k(q_kR_k,q_k\rho)\cdot\mathrm{A}_{\overline{1,2k}}],R_{k-1}<r<\rho<R_k\tag{35}$$

$$\mathcal{H}^*_{\nu\alpha_{k,n+1}}(p,r,\rho)=-\frac{q_{n+1}^{2\alpha_{n+1}}}{\Delta^*_{\nu\alpha}(p)\cdot\Delta_{\nu\alpha_{11}}}\prod_{s=k}^{n}\frac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}\Phi^{n+1}_{\nu\alpha_{11}}(q_{n+1}\rho,q_{n+1}R_{n+1})\left[\Phi^{k-1}_{\nu\alpha_{22}}(q_kR_{k-1},q_kr)\Delta_{\overline{1,2k-2}}-\Phi^{k-1}_{12}(q_kR_{k-1},q_kr)\Delta'_{\overline{1,2k-2}}\right]$$

$$\mathcal{H}^*_{n+1,n+1}(p,r,\rho)=\frac{q_{n+1}^{2\alpha_{n+1}}}{\Delta^*_{\nu\alpha}(p)}\begin{cases}\Phi^{n+1}_{11}(q_{n+1}\rho,q_{n+1}R_{n+1})\left[\Phi^{n}_{12}(q_{n+1}R_n,q_{n+1}r)\Delta'_{\overline{1,2n}}-\Phi^{n}_{22}(q_{n+1}R_n,q_{n+1}r)\Delta_{\overline{1,2n}}\right],R_n<\rho<r<R_{n+1}\\ \Phi^{n+1}_{11}(q_{n+1}r,q_{n+1}R_{n+1})\left[\Phi^{n}_{12}(q_{n+1}R_n,q_{n+1}\rho)\Delta'_{\overline{1,2n}}-\Phi^{n}_{22}(q_{n+1}R_n,q_{n+1}\rho)\Delta_{\overline{1,2n}}\right],R_n<r<\rho<R_{n+1}.\end{cases}$$

The functions $\mathcal{R}^*_{1_{k,j}}(p,z);k=\overline{1,n+1};j=\overline{1,n}$ of the influence of inhomogeneities of the first condition of the j-th interface $\omega_{1_j},j=\overline{1,n}$ on the kth segment of the adsorption medium are as follows:

$$\mathcal{R}^*_{1_{1j}}(p,r)=-\frac{1}{\Delta^*_{\nu\alpha}(p)}\begin{cases}\Phi^0_{\nu\alpha_{12}}(q_1R_0,q_1r)\mathrm{A}_{\overline{1,2}}; & j=1\\ \prod\limits_{s=1}^{j-1}\frac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}\cdot\Phi^0_{\nu\alpha_{12}}(q_1R_0,q_1r)\mathrm{A}_{\overline{1,2j}}; & j=\overline{2,n-1}\\ \prod\limits_{s=1}^{n-1}\frac{-c_{2_s}}{q_{s+1}^{2\alpha_{s+1}}R_s^{2\alpha_{s+1}+1}}\cdot\Phi^0_{\nu\alpha_{12}}(q_1R_0,q_1r)\Delta_{\nu\alpha_{11}}(q_{n+1}R_n,q_{n+1}R_{n+1}); & j=n\end{cases}\quad(36)$$

To obtain final analytical solutions that define a detailed mathematical model, it is necessary to perform the transition from images to originals. This is done in the following way. The singular points of the main solutions of the boundary value problem (6) - (8) $W^*_{1_k}(p,r),W^*_{n+1_k}(p,r),\mathcal{R}^*_{1_{kj}}(p,r),\mathcal{R}^*_{2_{kj}}(p,r),\mathcal{H}^*_{\nu\alpha_{k,k_1}}(p,r,\rho)$ are the branch points $p=\infty$ and

$$p_{1,2}=-\frac{1}{2}\left[S_1\pm\sqrt{S_2}\right]<0;$$
$$S_1=\beta_k(1+\gamma_k)+\eta_k^2;S_2=(\eta_k-\beta_k\gamma_k)^2=\beta_k\left[\beta_k(1+2\gamma_k)+2\eta_k^2\right]>0\,.\quad(37)$$

So, when passing to the Laplace originals, the integral over the Bromwich contour can be replaced by an integral over the imaginary axis

$$W_{1_k}(t,r)=L^{-1}\left[W^*_{1_k}(p,r)\right]=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}W^*_{1_k}(p,r)\cdot e^{pt}dp=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}W^*_{1_k}(p,r)\cdot e^{pt}dp=$$
$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}W^*_{1_k}(is,r)\cdot e^{ist}ds=\frac{1}{\pi}\int_0^{\infty}\mathrm{Re}\left[W^*_{1_k}(is,r)\cdot e^{ist}\right]ds;$$
$$W_{n+1_k}(t,r)=L^{-1}\left[W^*_{n+1_k}(p,r)\right]=\frac{1}{\pi}\int_0^{\infty}\mathrm{Re}\left[W^*_{n+1_k}(is,r)\cdot e^{ist}\right]ds;$$
$$R_{1_{kj}}(t,r)=L^{-1}\left[\mathcal{R}^*_{1_{kj}}(p,r)\right]=\frac{1}{\pi}\int_0^{\infty}\mathrm{Re}\left[\mathcal{R}^*_{1_{kj}}(is,r)\cdot e^{ist}\right]ds;\quad(38)$$
$$R_{2_{kj}}(t,r)=L^{-1}\left[\mathcal{R}^*_{2_{kj}}(p,r)\right]=\frac{1}{\pi}\int_0^{\infty}\mathrm{Re}\left[\mathcal{R}^*_{2_{kj}}(is,r)\cdot e^{ist}\right]ds;$$
$$\mathcal{H}^*_{k,k_1}(t,r,\rho)=L^{-1}\left[\mathcal{H}^*_{k,k_1}(p,r,\rho)\right]=\frac{1}{\pi}\int_0^{\infty}\mathrm{Re}\left[\mathcal{H}^*_{k,k_1}(is,r,\rho)\cdot e^{ist}\right]ds.$$

As a result of the unique solution of the algebraic system (25), taking into account the obtained main solutions of problem (6)-(8) and formulas (38), we obtain a unique solution to the original boundary value problem (1)-(5):

$$C_k(t,r)=\int_0^t W_{1_k}(t-\tau,r)\cdot\omega_{R_0}(t)d\tau+\int_0^t W_{n+1_k}(t-\tau,r)\cdot\omega_{R_{n+1}}(t)d\tau+$$
$$+\sum_{j=1}^{n}\int_0^t\left[\mathcal{R}_{1_{kj}}(t-\tau,r)\cdot\omega_{1_j}(\tau)+\mathcal{R}_{2_{kj}}(t-\tau,r)\cdot\omega_{2_j}(\tau)\right]d\tau+$$
$$+\int_0^t\sum_{k_1=1}^{n+1}\int_{R_{k_1-1}}^{R_{k_1}}\mathcal{H}_{k,k_1}(t-\tau;r,\rho)\cdot\left[f_{k_1}(\tau,\rho)+C_{0_{k_1}}(\rho)\cdot\delta_+(\tau)\right]\rho^{2a_{k_1}}d\rho d\tau+ \tag{39}$$
$$+\int_0^t\sum_{k_1=1}^{n+1}\int_{R_{k_1-1}}^{R_{k_1}}\frac{\beta_{k_1}\gamma_{k_1}}{D_{z_{k_1}}}\mathcal{H}_{k,k_1}(t-\tau;r,\rho)\,e^{-\beta_{k_1}\cdot\gamma_{k_1}\cdot\tau}\cdot a_{0_{k_1}}(\rho)\rho^{2a_{k_1}}d\rho d\tau;$$
$$a_k(t,z)=\beta_k\int_0^t e^{-\beta_k\gamma_k(t-\tau)}\cdot C_k(\tau,z)d\tau+e^{-\beta_k\gamma_k t}\cdot a_{0_k}(z).$$

In the expressions (39) the following designations are made:

$$\omega_1(t)=L\left[\omega_1^*(p)\right]=\omega_0(t)+(\delta_{11}^0\frac{d}{dr}+\gamma_{11}^0)C_{0_1}(r)\Big|_{r=R_0}\cdot\delta_+(t);$$
$$\omega_{l_{n+1}}(t)=L\left[\omega_{l_{n+1}}^*(p)\right]=\omega_{n+1}(t)+(\delta_{22}^{n+1}\frac{d}{dr}+\gamma_{22}^{n+1})C_{0_{n+1}}(r)\Big|_{r=R_0}\cdot\delta_+(t); \quad . \tag{40}$$
$$\omega_{mj}=\left[(\delta_{m1}^j\frac{d}{dr}+\gamma_{m1}^j)\cdot C_{0_j}(r)-(\delta_{m2}^j\frac{d}{dr}+\gamma_{m2}^j)C_{0_{j+1}}(r)\right]\Bigg|_{r=R_j}\cdot\delta_+(t);m=\overline{1,2};j=\overline{1,n}.$$

In order to describe the distribution of the electric field created by charged particles, which is formed inside the layered structure under study, we use the Poisson equation, which has the form:

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\varphi(r,z,t)\right]+\frac{\partial^2\varphi(r,z,t)}{\partial z^2}=-\frac{Q(r,z,t)}{4\pi\varepsilon_0\varepsilon(r)}, \tag{41}$$

where the charge distribution in the structure is:

$$Q(r,z)=e\left[C_k(t,r)-a_k(t,z)\right], \tag{42}$$

and the permittivity of the system is now defined as follows:

$$\varepsilon(r)=\sum_{i=0}^{N}\varepsilon_{(i)}\left[\theta(r-r_{(i)})-\theta(r-r_{(i+1)})\right],\ r_{(N+1)}\to+\infty\ . \tag{43}$$

The solution of equation (41) is sought on a multidimensional grid, which is given in the following form [7, 8]:

$$\Omega_{klm}=\left\{(r,t,z):r_k=k\Delta r_k,z_l=l\Delta z_l,t_m=m\Delta t_m,\ k,l,m\in Z\ \right\}. \tag{44}$$

Taking into account the boundary interface conditions for the potential $\varphi(r,z,t)$ and components of the electric field:

$$\varphi_{(p)}(r,z,t)\Big|_{r=r_{(p)}-0}=\varphi_{(p+1)}(r,z,t)\Big|_{r=r_{(p)}+0};$$
$$\varepsilon_{(p)}\frac{\partial\varphi_{(p)}(r,z,t)}{\partial r}\Bigg|_{r=r_{(p)}-0}=\varepsilon_{(p+1)}\frac{\partial\varphi_{(p+1)}(r,z,t)}{\partial r}\Bigg|_{r=r_{(p)}+0}. \tag{45}$$

In addition, it is taken into account that there is no electric field outside the microstructure, which gives the following condition:

$$\varphi(r,z,t)\big|_{z\to0}=\varphi(r,z,t)\big|_{z\to+\infty}=0.. \tag{46}$$

Thus, the finite difference scheme for finding solutions to the Poisson equation acquires the following form:

$$
\begin{aligned}
&\varphi_{k,l,m} - \varphi_{k+1,l,m} = 0;\\
&\frac{2\varphi_{k,l,m} - \varphi_{k+1,l,m}}{\Delta r_k} + \frac{\varphi_{k,l-1,m} - 2\varphi_{k,l,m} + \varphi_{k,l+1,m}}{\Delta z_l} - \frac{Q_{k,l,m}}{4\pi\varepsilon_0\varepsilon_k} = 0;\\
&\varepsilon_k \varphi_{k-1,l,m} - (\varepsilon_k + \varepsilon_{k+1})\varphi_{k,l,m} + \varepsilon_{k+1}\varphi_{k+1,l,m} = 0;\\
&\varphi_{0,l,m} = \varphi_{N+1,l,m} = 0;\\
&Q_{0,l,m} = Q_{N+1,l,m} = 0.
\end{aligned} \tag{47}
$$

3. Discussion of the results

In order to implement the developed mathematical model, the concentration distributions were calculated using relations (39). For this, the technological parameters of the microstructure experimentally studied in the papers [9, 10] were used. The microstructure under study is created from films of materials $Al_2 0_3/SiO_2$. In our calculations, it was assumed that the film thickness $Al_2 0_3$ is 0.1 μm and for thickness SiO_2 is 0.09 μm.

In Figure 2 are shown the results of calculations of the concentration $C(t, r)$ for charged particles in the sample under study, as well as the cross section of the spatial dependence of the plane, which more demonstrates the radial distribution of particles in the layers of the microstructure.

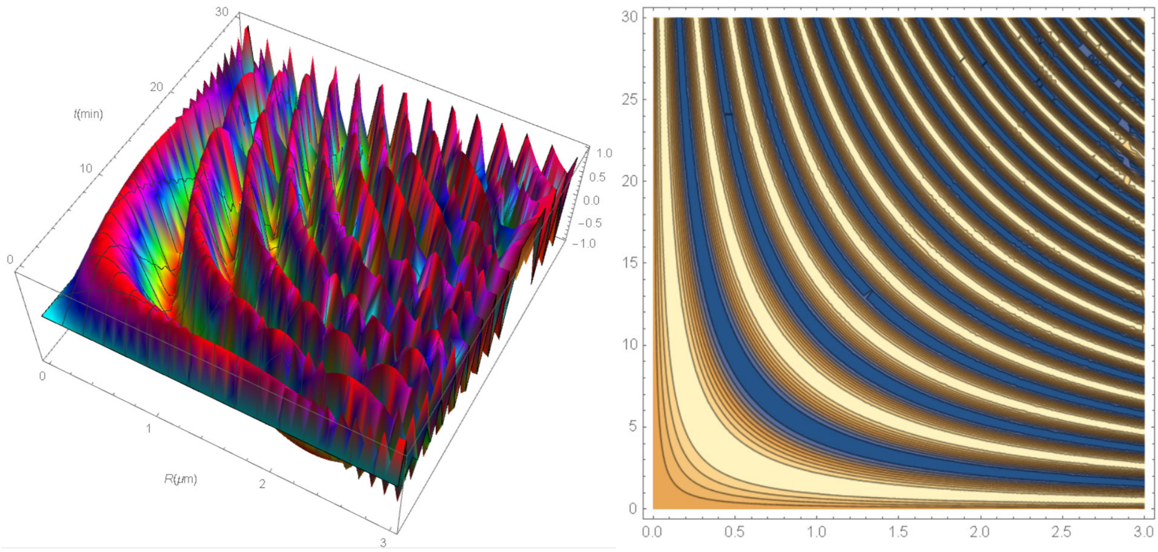

Figure 2: Spatial dependence of the concentration of charged particles in the intercrystalite space and the cross section of this dependence

Dependencies shown in Figure 2 demonstrate the concentration distribution of charged particles in the microstructure, which is formed by 15 layers of $Al_2 0_3$ and 16 layers of SiO_2. As can be seen from the figure, during a given time interval (up to 30 minutes), charged particles accumulate in the layers of the microsystem in such a way that they are contained mainly in the layers of the $Al_2 0_3$ material (light stripes), in contrast to the layers of SiO_2 where particles do not actually accumulate.

Further in Figure 3 are shown the results of calculating the concentration in the micropores of the layers of the studied microscopic sample. As can be seen from the calculated dependences, the concentration of charged frequencies in micropores is less than in the intercrystalite space, which is evidence that further filling of pores with particles is impossible. This is a sign of the achievement of phase equilibrium between the substance in the intercrystalite space of the microstructure layers and the substance in the pores. It should be noted that the cross section of the spatial dependence by a plane for this dependence is actually similar to the dependence shown in Figure 2 with the difference that the concentration increase does not occur immediately, but approximately 10 minutes after the adiabatic start of the process.

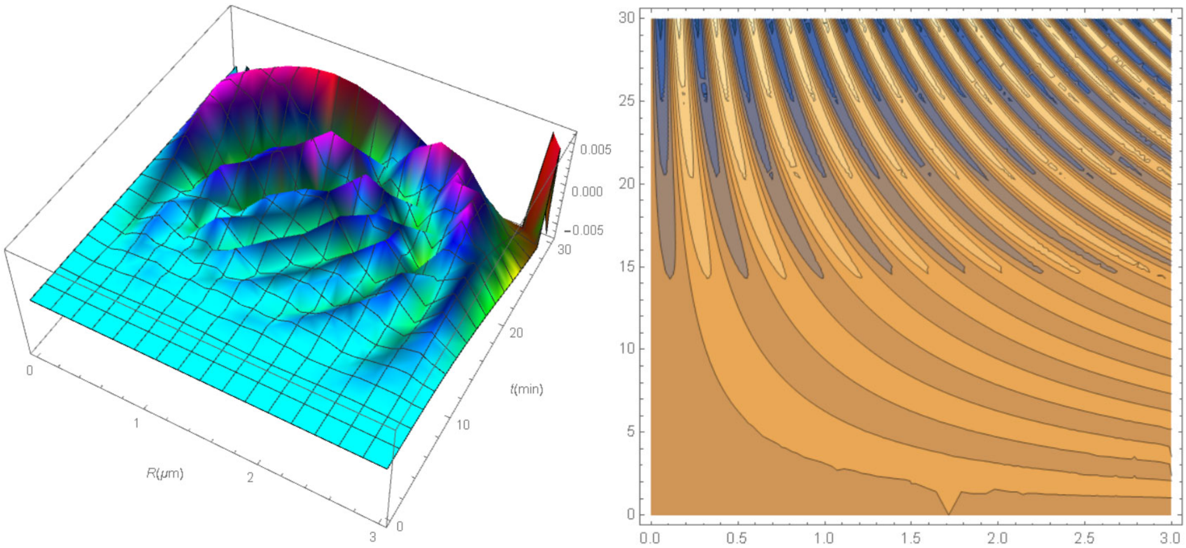

Figure 3: Spatial dependence of the concentration of charged particles in the porous space and the cross section of this dependence

Further, Figure 4 shows the result of calculating the spatial electrostatic potential created inside the microstructure by the charges accumulated in it. As can be seen from the calculated dependence, the electric field actually exists only inside the layers, which are mainly filled with charged particles. At the boundaries of the layers formed Al203 and SiO2, the potential of the electric field drops significantly and rapidly.

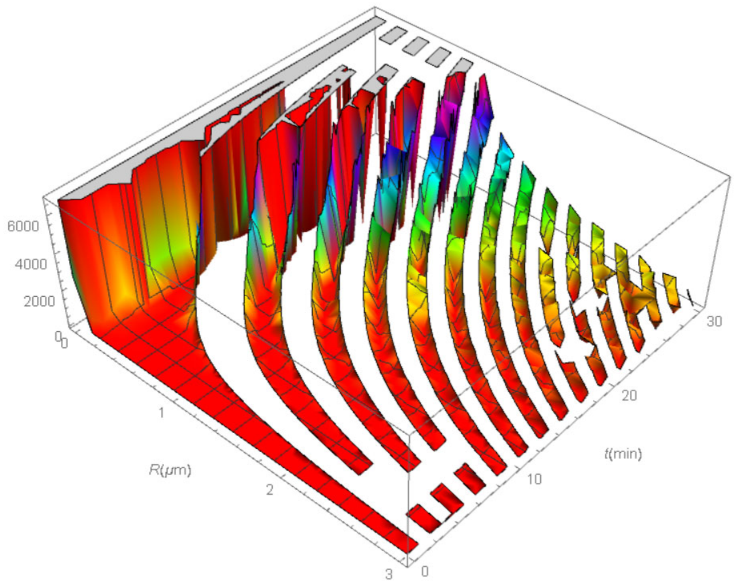

Figure 4: Spatial dependence of the electric field potential inside the studied microstructure

4. Concussions

In the proposed paper, a mathematical model of adsorption mass transfer in a limited cylindrical layered microporous medium is developed and analytical solutions are obtained for the first time, which generally describe the influence of factors of the internal kinetics of charged particle transfer, the main among which is the influence of non-stationary conditions of the system of n-interface relationships. . This makes it possible to model and build graphical concentration profiles of the adsorbate in macro- and micropores, to calculate the distribution of the electric potential inside the studied sample, to carry out a comprehensive analysis of the internal kinetics of mass transfer both at the macro level and at the level of micro- and nanopores of adsorbent particles, design optimal technological schemes and investigate for optimality various non-stationary modes of diffusion-adsorption mass transfer for multi-complex adsorption media with different physic-chemical conditions. The obtained model solutions and effective recurrent matrix algorithms for constructing matrices of influence functions of the boundary mass transfer problem are important in formulating and solving inverse mass transfer problems - to determine the kinetic parameters of the process, which makes it possible to check the adequacy of the modeling parameters and physical experiment.

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