Simulation of the Process of Water Purification in Multilayered Micro Porous Media

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Abstract— **The mathematical model of the process of adsorption purification of water from impurities in multilayer microporous filters is formulated. An algorithm for numerically-asymptotic approximation of solution of the corresponding nonlinear singularly perturbed boundary value problem is developed. The developed model allows to investigate the distribution of concentration of pollutant inside the filer.**

Keywords— mathematical model, process of water purification, micro porous media.

I. Introduction

Although a technological process of filtration with multi-layered filters with micro porous filling is widespread in industry, very few studies have systematically quantified its mechanism, and even less have characterized the affect of its parameters on operating costs and the quality of the final product. Sorption processes in zeolite catalysts are using in the technologies of separation and purification of gases in the chemical and petroleum industries, environmental engineering, etc. Fuller microporous adsorbents can be used in water treatment technological schemes, given their sorption properties [6, 8], as downloading multilayer filters using the principle of filtration in the direction of decreasing size microporous sorbent particles. In [1-4] the mathematical modeling of mass transfer problems of different nature in porous media without the internal structure of porous particles were explored. The problem of modeling the processes of diffusion and adsorption in microporous media and the problem of identification of kinetic parameters of these processes devoted significant number of publications [5-11]. The difficulty of theoretical description of the properties of micro porous heterogeneous environments from a mathematical point of view is the fact that the physical processes in such environments are described singularly perturbed boundary value, which coefficients are rapidly changing to different components within the section of the material. So important is the question of the development and application of new methods and approaches to modeling processes multicomponent mass transfer in heterogeneous microporous media if the prevalence of some components of the process over the other, leaning against a database of advanced physical experiments for these environments, which leads to a small parameter in the relevant members of equations. This work formed the component mathematical model of convection-diffusion mass transfer taking into account the mass exchange generated transfer pollution from interparticle space in internally lobed in multi-layer filter, consisting of different size and sorption properties of microporous particles.

II. Mathematical model

Consider the problem of modeling the process of mass transfer of pollutants in piecewise homogeneous multilayer microporous water-saturated media $G_{\mathbf{z}} = ABCDA_*B_*C_*D_*$. The environment is characterized by different filtering coefficients $\kappa=\left\{\kappa_j, (x,y,z)\in G_{\mathbf{z}}^j,\ j=\overline{1,m}\right\}$, the active porosity $\sigma=\left\{\sigma_j, (x,y,z)\in G_{\mathbf{z}}^j,\ j=\overline{1,m}\right\}$ and diffusion of pollutant $D=\left\{D_j=d_j\cdot\varepsilon, (x,y,z)\in G_{\mathbf{z}}^j,\ j=\overline{1,m}\right\}$, and each of the subregions consist of microporous particles of different sizes ($R=\left\{R_j,(x,y,z)\in G_{\mathbf{z}}^j,\ j=\overline{1,m}\right\}$ – the radius of particles in j th layer) and structure, characterized by porosity coefficients $\sigma^* = \left\{\sigma_j^*, (x,y,z)\in G_z^j,\ j=\overline{1,m}\right\}$, diffusion in micro particles $D^* = \left\{D_{i,j}^* = d_{i,j}^*\cdot\varepsilon, (x,y,z)\in G_z^j,\ j=\overline{1,m}\ i=\overline{1,k}\right\}$, influence of mass transfer coefficients $S=\left\{S_j=s_j\cdot\varepsilon, (x,y,z)\in G_{\mathbf{z}}^j,\ j=\overline{1,m}\right\}$ and adsorption equilibrium

$k=\{k_j,(x,y,z)\in G_z^j,\ j=\overline{1,m}\}$, where κ_j, σ_j, d_j, σ_j^*, d_j^*, s_j – some real positive numbers, ε – small parameter. The corresponding model problem in $G_z\times(0,R_j)\times(0,\infty)$ describes by equations:

$$\vec{v}=\kappa\cdot grad\,\varphi,\ div\,\vec{v}=0, \quad (1)$$

$$div(D\cdot grad\,\tilde{c})-\vec{v}\cdot grad\,\tilde{c}-S\,\tilde{q}'_r\big|_{r=R}=\sigma\tilde{c}'_t, \quad (2)$$

$$D^*(\tilde{q}''_{rr}+\frac{2}{r}\tilde{q}'_r)=\sigma^*\tilde{q}'_t \quad (3)$$

with initial and boundary conditions:

$$\varphi\big|_{ABB_*A_*}=\varphi_*,\ \varphi\big|_{CDD_*C_*}=\varphi^*,\ \frac{\partial\varphi}{\partial\vec{n}}\Big|_{ADD_*A_*\cup BCC_*B_*\cup ABCD\cup A_*B_*C_*D_*}=0, \quad (4)$$

$$\tilde{c}\ (x,y,z,t)\big|_{t=0}=\tilde{c}^0(x,y,z),\ \tilde{c}\ \big|_{ABB_*A_*}=\tilde{c}_*(M,t),$$
$$\tilde{c}\big|_{CDD_*C_*}=\tilde{c}^*(M,t),\ \tilde{c}\ \big|_{BCC_*B_*}=\tilde{c}_{**}(M,t),\ \tilde{c}\ \big|_{ADD_*A_*}=\tilde{c}^{**}(M,t),$$
$$\tilde{c}\ \big|_{ABCD}=\tilde{c}_{***}(M,t),\ \tilde{c}\ \big|_{A_*B_*C_*D_*}=\tilde{c}^{***}(M,t), \quad (5)$$
$$\tilde{q}(x,y,z,r,t)\big|_{t=0}=\tilde{q}^0(x,y,z,r),\ \tilde{q}(x,y,z,r,t)\big|_{r=R}=k\,\tilde{c}(x,y,z,t),$$
$$\frac{\partial\,\tilde{q}(x,y,z,r,t)}{\partial\,r}\bigg|_{r=0}=0$$

and terms of consistency in equipotential surface the surface of the layer section:

$$\varphi\ \big|_{E_jF_jF_{*j}E_{*j-}}=\varphi\ \big|_{E_jF_jF_{*j}E_{*j+}}=\varphi_{*j}^*,$$
$$\kappa_j\cdot\varphi'_{\vec{n}}\big|_{E_jF_jF_{*j}E_{*j-}}=\kappa_{j+1}\cdot\varphi'_{\vec{n}}\big|_{E_jF_jF_{*j}E_{*j+}}, \quad (6)$$
$$\tilde{c}\big|_{E_jF_jF_{*j}E_{*j-}}=\tilde{c}\big|_{E_jF_jF_{*j}E_{*j+}},$$
$$\left(D_j\frac{\partial\tilde{c}}{\partial\vec{n}}-v_n^j\tilde{c}\right)\bigg|_{E_jF_jF_{*j}E_{*j-}}=\left(D_{j+1}\frac{\partial\tilde{c}}{\partial\vec{n}}-v_n^j\tilde{c}\right)\bigg|_{E_jF_jF_{*j}E_{*j+}}. \quad (7)$$

Here $\tilde{c}_j(x,y,z,t)$ is concentration of pollutant in j th layer of filter, and $\tilde{q}_j(x,y,z,r,t)$ concentration of pollutant particles in filter, φ and $\vec{v}(v_x,v_y,v_z)$ is respectively potential (quasipotential) and vector filtration rate ($0<\varphi_*\le\varphi\le\varphi^*<\infty$, $|\vec{v}|=\sqrt{v_x^2(x,y,z)+v_y^2(x,y,z)+v_z^2(x,y,z)}>v_*>>0$), φ_* , φ^* – arbitrary real positive numbers, $\vec{n}$ – external normal to the respective surface, M is arbitrary point of corresponding surface v_n^j is normal components of velocity on the appropriate interface $E_jF_jF_{*j}E_{*j}$ ($j=\overline{1,m-1}$), φ_{*j}^* – unknown value potential for the respective interface $E_jF_jF_{*j}E_{*j}$, $0<\varphi_*<\varphi_{*1}^*<\varphi_{*2}^*<\ldots<\varphi_{*m-1}^*<\varphi^*<\infty$. We assume that all the features that appear in conditions (4-6) are sufficiently smooth and coordinated with each other along the edges and corner points of the area as well as on surfaces $E_jF_jF_{*j}E_{*j}$ ($j=\overline{1,m-1}$) section of subdomains.

III. Methods

Take into account the relationship between the values of parameters that characterize certain components of the process (in particular the dominance of convective and mass-exchange components over diffusion) leads to the complication of the mathematical model of the process of singularities, which are generated by the presence of small parameters. One of the effective ways of solving the corresponding problems in the case of the predominance of convective components of the process over diffusion during filtration of aqueous solutions in the model regions limited by equipotential or quasi-quipotential lines and flow lines is: phased fixation of the characteristics and components of the process and environment; solving filtration problems using conformal or quasiconformal mappings of a complex potential or quasipotential area on a physical area; transition in equations of convective diffusion and boundary and initial conditions from physical variables to the coordinates of the region of complex potential or quasipotential, which greatly simplifies their recording and provides the possibility of autonomous research, parallel computing.

Taking into account that the problem is to find the velocity field (1) with the given boundary conditions (4), (6) is resolved [5], in particular, calculated velocity field and a number of other variables, such as filtration consumption, and replaced the $x=x(\varphi,\psi,\chi)$, $y=y(\varphi,\psi,\chi)$, $z=z(\varphi,\psi,\chi)$ in the system (2)-(3) and conditions (5)-(7), received the corresponding "diffusion problem" [3-5], which solution with precision found in the form of asymptotic series [5].

IV. Results of numerical calculations

Effect of physical and chemical properties of microparticles to distribution of concentration of pollutant in G_z^1 [5] illustrated in figure 1-3. In particular, the results describe the influence factor of internally particulate transfer to interparticle the first subregion (figure 1) and the coefficient of adsorption equilibrium in the first subregion $K_1=0.8$ (figure.2) for the distribution of pollutant concentrations in the interparticle space in the following inputs:
$\kappa_1=0.45\,m/day$, $\kappa_2=0.3\,m/day$, $\sigma_1=\sigma_2=0.7$, $D_1=D_2=0.008\,m^2/day$, $D_1^*=10^{-8}m^2/day$, $D_2^*=10^{-6}m^2/day$, $K_2=0.9$, $S_2=0.005$, $\sigma_1^*=\sigma_2^*=0.3$, $R_1=R_2=10^{-5}m$.

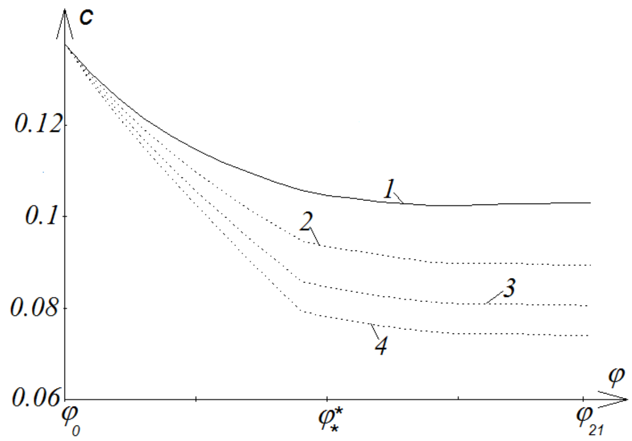

Figure 1. Influence of internally particulate transfer to interparticle

The solid curve figure 1, 2 corresponds the convective component process (no influence diffusion and adsorption micro porous particles), curve 1 corresponds to the figure 1

$S_1 = 0.005$ curve 2 – $S_1 = 0.009$, curve 3 – $S_1 = 0.012$, and the figure 2, curve 1 corresponds to the $K_1 = 0.4$, curve 2 – $K_1 = 0.65$, curve 3 – $K_1 = 0.87$ along the flow $(\varphi, \psi_4, \chi_4)$ at time $t = 15\ day$.

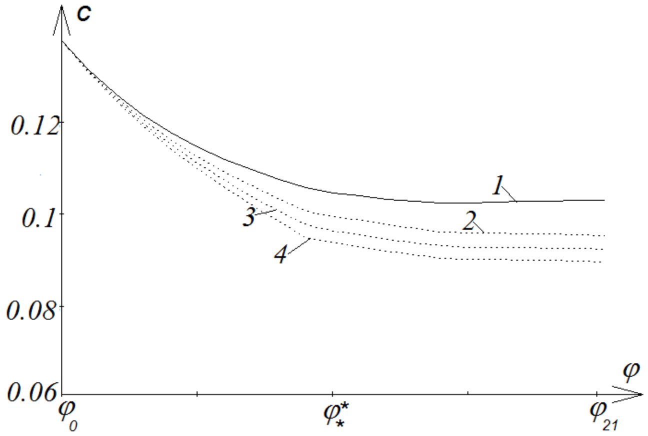

Figure 2. Influence of the coefficient of adsorption equilibrium in the first subregion

On figure 3 illustrates the effect of diffusion and adsorption on the distribution of pollutant concentrations in the interparticle space. Curves 1 - 3 correspond to the convective component solution $c_{j,0}(\varphi, \psi_4, \chi_4, t)$, and curves 1* - 3* – the solution $c_{j,1}(\varphi, \psi_4, \chi_4, t)$ in accordance times $t = 1\ day$, $t = 8\ days$ and $t = 15\ days$ according to such initial and boundary conditions:

$$c_1^0(\varphi,\psi,\chi) = c_2^0(\varphi,\psi,\chi) = 0.15 + 0.02\left(\frac{\varphi_0^2 - \varphi^2}{100} + 1\right) tg\left(\frac{\psi^2 + \chi^2}{100}\right),$$

$$c_1^0(\varphi,\psi,\chi) = c_2^0(\varphi,\psi,\chi) = 0.1 + 0.01\left(\frac{\varphi_0^2 - \varphi^2}{100} + 1\right) tg\left(\frac{\psi^2 + \chi^2}{100}\right),$$

$$c_{1*}(\psi,\chi,t) = 0.15 + 0.02 tg\left(\frac{\psi^2 + 5t + \chi^2}{100}\right),$$

$$c_{2*}(\psi,\chi,t) = 0.1 + 0.01 tg\left(\frac{\psi^2 + 10t + \chi^2}{100}\right),$$

$$q_j^0(\varphi,\psi,\chi,r) = K_j\left(\frac{2}{\pi} arctg\left(\frac{100(r - R_j)}{R_j}\right) + 1\right) c_j^0(\varphi,\psi,\chi).$$

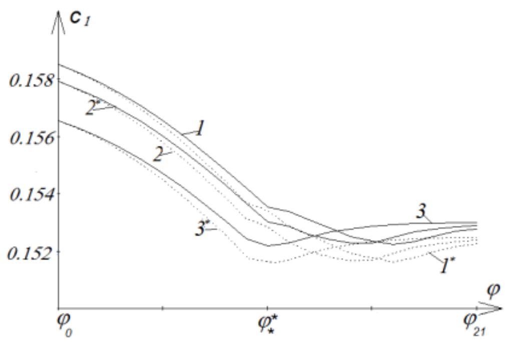

Figure 3. The effect of diffusion and adsorption on the distribution of pollutant concentrations in the interparticle space

Conclusions

The paper presents a mathematical model of the singularly perturbed process of convection-diffusion mass transfer of soluble substances in the heterogeneous microporous filter and obtained asymptotic expansions of solutions of the corresponding boundary problems. Confirmed that despite the low rate of diffusion mass transfer phenomena in the pores of the particles, eventually it significantly affects the distribution of concentration in particles and in all the filter, and thus it is possible to use considered microporous media to cleaning fluids from contamination. The algorithms and software procedures allows to take into account the structure and characteristics of the environment, especially the transfer on micro and macro level, technological parameters that are necessary for optimum purification process setting using microporous adsorbents for obtaining the required quality of output products and optimal usage of microporous filling of filters.

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