

# Identification of mass-transfer coefficient in spatial problem of filtration

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A modeling problem of the process of liquid multi component decontamination by a spatial filter is considered, it takes into account the reverse influence of decisive factors (contamination concentrations of liquid and sediment) on characteristics (coefficient of porosity, diffusion) of the medium and gives us the possibility to determine small mass transfer coefficient under the conditions of prevailing of convective constituents over diffusive ones. An algorithm of the solution of the corresponding nonlinear singular disturbed inverse problem of "convection-diffusion mass transfer" type is suggested.

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#### 1. Introduction

Analysis of results of researches [1–15] testifies to the presence of complex structure of interdependence of different factors which determine the processes of filtration and filtering through porous media and were not taken into account in the traditional (classic, phenomenological) models of such systems. The reason for the construction of mathematical models of processes of liquid multi component decontamination by a spatial filter is the absence of "model mechanisms" that take into account the inverse influence of different kinds of process characteristics on environment and identification of unknown parameters that are included into the corresponding models.

In work [10], the mathematical model of process of liquid purification is worked out in porous filter nozzle that takes into account reverse influence of characteristics of process (concentrations of sediment) on filtration parameters, herewith some coefficients of the considered process, were determined in experimental way.

In this work, the mathematical model is constructed of filtration process of liquid from multi component contamination in a spatial filter taking into account the unknown small mass transfer coefficient under the conditions of prevailing of convective constituents over diffusive. The solution of the corresponding inverse problem gives us an opportunity to approach substantially the numerical calculations to the experimental data (in comparison to the classic phenomenological models [13]), more exactly to predict and calculate the efficiency of process of precipitation of impurities of the different technological water-dispersible systems.

### 2. Statement of the problem

Let us consider the curvilinear parallelepiped (filter) of  $G_z = ABCDA_*B_*C_*D_*$ , bounded by smooth orthogonal equipotential surfaces between themselves at angular points and edges

$$ABB_*A_* = \{z : f_1(x, y, z) = 0\}, \quad CDD_*C_* = \{z : f_2(x, y, z) = 0\}$$

and also surfaces of flow

$$ADD_*A_* = \{z : f_3(x, y, z) = 0\}, \quad BCC_*B_* = \{z : f_4(x, y, z) = 0\},$$
  
 $ABCD = \{z : f_5(x, y, z) = 0\}, \quad A_*B_*C_*D_* = \{z : f_6(x, y, z) = 0\}.$ 

Assume [10] that the contamination particles of substance impurities can transfer from one state to another (processes of entrapping-releasing, sorption-desorption), herewith the concentrations of contamination influence on characteristics of corresponding medium (porosity, coefficient of filtration, and others like that). The concentration of contamination is multi component  $(C = C(x, y, z, t) = (C_1, \ldots, C_m))$ , where  $C_i$  is the concentration of *i*-th impurity component  $(i = \overline{1, m})$  in the liquid filter medium. The corresponding process of filtration for the domain of  $G = G_z \times (0, \infty)$  is described by the following modeling problem:

$$\begin{cases}
\frac{\partial (\sigma(P)C_{i})}{\partial t} = \varepsilon \alpha(t) P - \overrightarrow{v} \cdot \overrightarrow{\nabla} C_{i} - \beta_{i} \sum_{p=1}^{m} q_{p}C_{p} - \\
-\varepsilon f_{m-1} \left( \sum_{p_{1}, \dots, p_{u}=1}^{m} h_{i, p_{1}, \dots, p_{u}} C_{i}^{\gamma_{i}} C_{p_{1}}^{\gamma_{p_{1}}} \dots C_{p_{u}}^{\gamma_{p_{u}}} \right) + D_{i} \Delta C_{i}, \\
\frac{\partial P}{\partial t} = \left( \sum_{i=1}^{m} \beta_{i} C_{i} \right) - \varepsilon \alpha(t) P, \ i = \overline{1, m},
\end{cases} \tag{1}$$

$$C_{i}\left|_{ABB_{*}A_{*}}\right.=C_{i,*}\left(M,t\right),\quad \left.\frac{\partial C_{i}}{\partial \,\overrightarrow{n}}\right|_{CDD_{*}C_{*}}=0,\quad \left.\frac{\partial C_{i}}{\partial \,\overrightarrow{n}}\right|_{ADD_{*}A_{*}\cup BCC_{*}B_{*}\cup ABCD\cup A_{*}B_{*}C_{*}D_{*}}=0,$$

$$C_{i}(x, y, z, 0) = C_{i,0}^{0}(x, y, z), P(x, y, z, 0) = P_{0}^{0}(x, y, z),$$
 (2)

$$\overrightarrow{v} = \kappa(P) \nabla \varphi, \ \nabla \cdot \ \overrightarrow{v} = 0, \tag{3}$$

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

$$\alpha(t) \iiint\limits_{G} P(\tilde{x}, \tilde{y}, \tilde{z}, t) d\tilde{x} d\tilde{y} d\tilde{z} = \mu(t), \tag{5}$$

where P(x, y, z, t) is the concentration of the sediment in the internal point (x, y, z) of the domain G (loading of filter) at the instant of time of t;  $\beta_i$  are the coefficients which characterize the mass volumes of besieging of impurities per time unit,  $\alpha(t)$  is unknown coefficient which characterizes mass volumes of the particles torn off from the granules of loading,  $\mu(t)$  is the function which characterizes mass distributing of sediment in the course of time (it is determined by an experimental method [13]) (5) is a condition of redetermination;  $\sigma(P)$  is the porosity of medium  $(\sigma(P) = \sigma_0 - \varepsilon \sigma_* P(x, y, z, t))$ ;  $\overrightarrow{\nabla}$  is the operator of Hamilton;  $\Delta = \overrightarrow{\nabla} \cdot \overrightarrow{\nabla}$  is the operator of Laplace;  $D_i = d_{0i}\varepsilon$  is the coefficient

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of diffusion of impurity in the liquid;  $\sigma_*$ ,  $d_{0i}$ ,  $\varepsilon$  are hard parameters (characterize the corresponding soft parameter  $\sigma(P)$ ) which are determined by an experimental method,  $\varepsilon$  is the small parameter (it characterizes advantages of one components of process over others, namely, desorptional components and phenomenon of component interaction of this process are small in comparison with other its components);  $C_i^*(M,t)$ ,  $C_{i,0}^0(x,y,z)$  are smooth enough functions coherent between themselves on the edges of domain G; M is an arbitrary point of corresponding surface;  $\varphi$  is the filtration potential  $(0 < \varphi_* \le \varphi \le \varphi^* < \infty)$ ;  $\overrightarrow{v}(v_x, v_y, v_z)$  is the vector of filtration rate  $(|\overrightarrow{v}| > v_* \gg \varepsilon)$ ;  $\kappa = K(P)$  is the coefficient of filtration of corresponding porous medium (K(P)) is the given, sufficiently smooth function);  $\overrightarrow{n}$  is the external normal to the corresponding surface.

By the method of introduction of the pair of the functions,  $\psi = \psi(x, y, z)$ ,  $\eta = \eta(x, y, z)$  (spatially quasi-complex conjugated with the function  $\varphi(x, y, z)$ ) such that  $\kappa \cdot \operatorname{grad} \varphi = \operatorname{grad} \psi \times \operatorname{grad} \eta$  [10] and substituting the boundary conditions:  $\psi|_{ADD_*A_*} = 0$ ,  $\psi|_{BCC_*B_*} = Q_*$ ,  $\eta|_{ABCD} = 0$ ,  $\eta|_{A_*D_*C_*B_*} = Q^*$ , this problem is replaced by more general direct problem of finding spatial analogue of quasi-conformal mapping the domain  $G_z$  on the corresponding domain of complex quasi-potential

$$G_w = \{ w = (\varphi, \psi, \eta) : \varphi_* \leqslant \varphi \leqslant \varphi^*, \ 0 < \psi < Q_*, \ 0 < \eta < Q^* \}$$

where,  $Q_*$ ,  $Q^*$  are unknown parameters,

$$Q_* \cdot Q^* = Q = \int_{EFF_*E_*} \frac{\partial \varphi}{\partial s} ds$$

amount of liquid that passes through some quasi-potentional surface  $EFF_*E_*$  of domain  $G_{\mathbf{z}}$  (complete filtration expense). We assume that this problem on a spatial conformal mapping  $G_w \mapsto G_z$  ( $G_w = \{w = (\varphi, \psi, \eta) : \overline{\varphi_*} < \varphi < \overline{\varphi^*}, \ 0 < \psi < Q_*, \ 0 < \eta < Q^*\}$  is corresponding  $G_z$  domain of complex potential) at some average value of  $\kappa$  was determined [9,10], in particular, dynamic net was built and field of filtration rate,  $\overrightarrow{v}$  filtration expense was calculated for  $Q = Q_*Q^*$ . Then, making out replacement of variables  $x = x \ (\varphi, \psi, \eta)$ ,  $y = y \ (\varphi, \psi, \eta)$ ,  $z = z \ (\varphi, \psi, \eta)$  in the system (1) and conditions (2), come to the corresponding problem for the domain of  $G_w \times (0, \infty)$ :

$$\begin{cases}
\frac{\partial (\sigma(\rho) c_{i})}{\partial t} = \varepsilon \alpha(t) \rho - v^{2} \frac{\partial c_{i}}{\partial \varphi} - \beta_{i} \sum_{p=1}^{m} q_{p} C_{p} - \varepsilon \sum_{p=1, i \neq p}^{m} h_{i,p} c_{i,j-1} c_{p,j-1} + \\
+ \varepsilon d_{0i} \left( v^{2} \frac{\partial^{2} c_{i}}{\partial \varphi^{2}} + b_{1} \frac{\partial^{2} c_{i}}{\partial \psi^{2}} + b_{2} \frac{\partial^{2} c_{i}}{\partial \eta^{2}} + d_{1} \frac{\partial c_{i}}{\partial \psi} + d_{2} \frac{\partial c_{i}}{\partial \eta} \right), \\
\frac{\partial \rho}{\partial t} = \sum_{i=1}^{m} \beta_{i} c_{i} - \varepsilon \alpha(t) \rho,
\end{cases} (6)$$

$$c_{i}(\bar{\varphi}_{*}, \psi, \eta, t) = c_{i}^{*}(\psi, \eta, t), \quad c_{i,\varphi}(\bar{\varphi}^{*}, \psi, \eta, t) = 0,$$

$$c_{i,\psi}(\varphi, 0, \eta, t) = c_{i,\psi}(\varphi, Q_{*}, \eta, t) = c_{i,\eta}(\varphi, \psi, 0, t) = c_{i,\eta}(\varphi, \psi, Q^{*}, t) = 0,$$

$$c_i(\varphi, \psi, \eta, 0) = c_{i,0}(\varphi, \psi, \eta), \quad \rho(\varphi, \psi, \eta, 0) = \rho_0(\varphi, \psi, \eta), \tag{7}$$

$$\alpha(t) \iiint_{G_w} \rho(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta} = \mu(t), \tag{8}$$

where (see, e.g. [9,10])

$$c_i = c_i (\varphi, \psi, \eta, t) = C_i (x(\varphi, \psi, \eta), y(\varphi, \psi, \eta), z(\varphi, \psi, \eta), t)$$

$$\begin{split} \rho &= \rho \left( \varphi, \psi, \eta, t \right) = P \left( x(\varphi, \psi, \eta), y(\varphi, \psi, \eta), z(\varphi, \psi, \eta), t \right), \\ b_1 &= b_1 \left( \varphi, \psi, \eta \right) = \left( \overrightarrow{\nabla} \psi \right)^2, \quad b_2 = b_2 \left( \varphi, \psi, \eta \right) = \left( \overrightarrow{\nabla} \eta \right)^2, \quad d_1 = d_1 \left( \varphi, \psi, \eta \right) = \Delta \psi, \\ d_2 &= d_2 \left( \varphi, \psi, \eta \right) = \Delta \eta, \end{split}$$

$$\begin{split} v^2\left(\varphi,\psi,\eta\right) &= v_x^2\left(x(\varphi,\psi,\eta),y(\varphi,\psi,\eta),z(\varphi,\psi,\eta)\right) + v_y^2\left(x(\varphi,\psi,\eta),y(\varphi,\psi,\eta),z(\varphi,\psi,\eta)\right) + \\ &\quad + v_z^2\left(x(\varphi,\psi,\eta),y(\varphi,\psi,\eta),z(\varphi,\psi,\eta)\right). \end{split}$$

### 3. Asymptotic nature of the solution

The solution of the problem (6), (8) with needed accuracy we search as asymptotic series [9,10]:

$$c_{i} = c_{i,0} + \sum_{j=1}^{n} \varepsilon^{j} c_{i,j} + \sum_{j=0}^{n} \varepsilon^{j} \Pi_{i,j} + \sum_{j=0}^{n} \varepsilon^{j} \bar{\Pi}_{i,j} + \sum_{j=0}^{n+1} \varepsilon^{j/2} \tilde{\Pi}_{i,j} + \sum_{j=0}^{n+1} \varepsilon^{j/2} \tilde{\Pi}_{i,j} + \sum_{j=0}^{n+1} \varepsilon^{j/2} \tilde{\Pi}_{i,j} + \sum_{j=0}^{n+1} \varepsilon^{j/2} \tilde{\Pi}_{i,j} + R_{c,i},$$

$$(9)$$

$$\rho = \rho_0 + \sum_{j=1}^n \varepsilon^j \rho_j + \sum_{j=0}^n \varepsilon^j P_j + \sum_{j=0}^n \varepsilon^i \bar{P}_j + \sum_{j=0}^{n+1} \varepsilon^{j/2} \tilde{P}_j +$$
(10)

$$+\sum_{j=0}^{n+1} \varepsilon^{j/2} \,\bar{\bar{P}}_j + \sum_{j=0}^{n+1} \varepsilon^{j/2} \,\tilde{\tilde{P}}_j + \sum_{j=0}^{n+1} \varepsilon^{j/2} \,\hat{P}_j + R_\rho, \tag{11}$$

$$\alpha(t) = \alpha_0(t) + \sum_{j=1}^{k} \varepsilon^j \alpha_j(t) + R_{\alpha}(t, \varepsilon), \qquad (12)$$

where  $R_{c,i}(\varphi, \psi, \eta, t, \varepsilon)$ ,  $R_{\rho}(\varphi, \psi, \eta, t, \varepsilon)$ ,  $R_{\alpha}(\varphi, \psi, \eta, t, \varepsilon)$  are remainder members,  $c_{i,j}(\varphi, \psi, \eta, t)$ ,  $\rho_{j}(\varphi, \psi, \eta, t)$ ,  $\alpha_{j}(t)$  are members of regular part of asymptotics  $(i = \overline{1, m}; j = \overline{0, n})$ ;  $\Pi_{i,j}(\xi, \psi, \eta, t)$ ,  $P_{j}(\xi, \psi, \eta, t)$  are functions of the boundary type for the layer in  $\varphi = \overline{\varphi}^{*}$  (corrections are made at the filter inlet)  $(j = \overline{0, 2})$ ,  $\overline{\Pi}_{i,j}(\overline{\xi}, \psi, \eta, t)$ ,  $\overline{P}_{j}(\overline{\xi}, \psi, \eta, t)$  in  $\varphi = \overline{\varphi}_{*}$  (corrections are made at the filter inlet)  $(j = \overline{0, 2})$ , and functions  $\widetilde{\Pi}_{i,j}(\varphi, \widetilde{\psi}, \eta, t)$ ,  $\overline{\overline{\Pi}}_{i,j}(\varphi, \overline{\psi}, \eta, t)$ ,  $\widetilde{\overline{\Pi}}_{i,j}(\varphi, \psi, \widetilde{\eta}, t)$ ,  $\widehat{\Pi}_{i,j}(\varphi, \psi, \widetilde{\eta}, t)$ ,  $\widehat{P}_{j}(\varphi, \psi, \widetilde{\eta}, t)$ ,

By the substitution of correlations (9)–(11) into (6)–(8) and fulfilling the standard procedure of "equating" of coefficients at identical degrees  $\varepsilon$ , we obtain the following problems to solve  $c_{i,j}(\varphi, \psi, \eta, t)$ ,  $\rho_j(\varphi, \psi, \eta, t)$   $(j = \overline{0, n})$ 

$$\begin{cases}
\sigma_0 \frac{\partial c_{i,0}}{\partial t} + v^2 \frac{\partial c_{i,0}}{\partial \varphi} + \beta_i c_{i,0} = 0, & \frac{\partial \rho_0}{\partial t} = \sum_{i=1}^m \beta_i c_{i,0}, \\
c_{i,0}(\varphi, \psi, \eta, 0) = c_{i,0}^0, & c_{i,0}(\varphi_*, \psi, \eta, t) = c_{i*}(\psi, \eta, t), \\
\rho_0(\varphi, \psi, \eta, 0) = \rho_0^0;
\end{cases}$$

$$\alpha_0(t) \iiint_C \rho_0(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta} = \mu(t),$$

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$$\begin{cases} -\sigma_*\rho_{j-1}\frac{\partial c_{i,j}}{\partial t} + v^2\frac{\partial c_{i,j}}{\partial \varphi} + \beta_i c_{i,j} + \sum_{l,g=1,\ l\neq g}^m k_{l,g}c_{l,j-1}c_{g,j-1} = U_{i,j}, \\ \frac{\partial \rho_j}{\partial t} = \sum_{i=1}^m \beta_i c_{i,j} - \sum_{k=1}^j \alpha_{j-k}(t)\rho_{k-1}, \\ c_{i,j}\left(\varphi,\psi,\eta,0\right) = 0, \quad c_{i,j}\left(\varphi_*,\psi,\eta,t\right) = 0, \\ \rho_j\left(\varphi,\psi,\eta,0\right) = 0; \end{cases}$$

$$\alpha_{0}(t) \iiint_{G_{w}} \rho_{0}(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta} + \alpha_{1}(t) \iiint_{G_{w}} \rho_{j-1}(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta} + \dots + \\ + \alpha_{j}(t) \iiint_{G_{w}} \rho_{0}(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta} = 0.$$

As a result of their solving, we obtain

$$\begin{split} c_{i,0} &= \left\{ \begin{array}{l} c_{i,*} \left( \psi, \eta, t - f \right) \exp \left[ -\beta_i \int\limits_{\varphi_*}^{\varphi} \frac{d\tilde{\varphi}}{v^2 \left( \tilde{\varphi}, \psi, \eta \right)} \right], \quad t \geqslant f, \\ c_{i,0} \left( f^{-1} \left( f - t, \psi, \eta \right), \psi, \eta \right) \exp \left[ -\frac{\beta_i t}{\sigma_0} \right], \quad t < f, \\ \rho_0 &= \int\limits_0^t \left( \sum_{i=1}^m \beta_i c_{i,0} \right) d\tilde{t} + \rho_0^0, \quad \alpha_0(t) = \frac{\mu(t)}{\iint\limits_{G_w} \rho_0(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta}}, \\ c_{i,j} &= \left\{ \begin{array}{l} e^{-\lambda_1} \int\limits_{\varphi_0}^{\varphi} \frac{U_{i,j} \left( s, \psi, \eta, f \left( s, \psi, \eta \right) - f + t \right)}{v^2 \left( s, \psi, \eta \right)} e^{\lambda_2 \left( s, \psi, \eta, t \right)} ds, \quad , t \geqslant f, \\ -\frac{e^{-\lambda_1}}{\sigma_*} \int\limits_0^t \frac{U_{i,j} \left( f^{-1} \left( s + f - t, \psi, \eta \right), \psi, \eta, s \right)}{\rho_{j-1} \left( f^{-1} \left( s + f - t, \psi, \eta \right), \psi, \eta, \eta \right)} e^{\lambda_2 \left( \varphi, \psi, \eta, s \right)} ds, \quad t < f, \\ \rho_j &= \int\limits_0^t \left( \sum_{i=1}^m \beta_i c_{i,j} - \sum_{k=1}^j \alpha_{j-k}(t) \rho_{k-1} \right) d\tilde{t}, \quad \alpha_j(t) &= \frac{\sum_{k=1}^j \alpha_{j-k}(t) \iint\limits_{G_w} \rho_j(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta}}{\iint\limits_{G_w} \rho_0(\tilde{\varphi}, \tilde{\psi}, \tilde{\eta}, t) d\tilde{\varphi} d\tilde{\psi} d\tilde{\eta}}, \end{split}$$

where

$$\begin{split} U_{i,j}\left(\varphi,\psi,\eta,t\right) &= d_{0i}\left(v^2\frac{\partial^2 c_{i,j}}{\partial \varphi^2} + b_1\frac{\partial^2 c_{i,j}}{\partial \psi^2} + b_2\frac{\partial^2 c_{i,j}}{\partial \eta^2} + d_1\frac{\partial c_{i,j}}{\partial \psi} + d_2\frac{\partial c_{i,j}}{\partial \eta}\right) + \\ &\quad + \alpha_{j-1}\left(t\right)\rho_{j-1} - \sum_{l,g=1,\ l\neq g}^{m} k_{l,g}c_{l,j-1}c_{g,j-1}, \qquad \left(j = \overline{2,n}\right), \end{split}$$
 
$$\lambda_1\left(\varphi,\psi,\eta,t\right) = -\beta_i\int\limits_{-\infty}^{\varphi} \frac{\rho_{j-1}\left(s,\psi,\eta,f\left(\tilde{\varphi},\psi,\eta\right) + t - f\right)c_{i,j}\left(s,\psi,\eta,f\left(\tilde{\varphi},\psi,\eta\right) + t - f\right)}{v^2\left(s,\psi,\eta\right)} \, ds, \end{split}$$

$$\lambda_{2}\left(\varphi,\psi,\eta,t\right) = -\beta_{i} \int_{0}^{t} \frac{\rho_{j-1}\left(f^{-1}\left(\tilde{s}+f-t,\psi,\eta\right),\psi,\eta,\tilde{s}\right)c_{i,j}\left(f^{-1}\left(\tilde{s}+f-t,\psi,\eta\right),\psi,\eta,\tilde{s}\right)}{\sigma\left(f^{-1}\left(\tilde{t}+f-t,\psi,\eta\right),\psi,\eta\right)} d\tilde{s},$$

$$f(\varphi,\bar{\psi},\bar{\eta}) = \int_{\varphi_{0}}^{\varphi} \frac{ds}{v^{2}\left(s,\bar{\psi},\bar{\eta}\right)}$$

is the time of transit of the corresponding particle way from the point

$$(x(\varphi_*, \bar{\psi}, \bar{\eta}), y(\varphi_*, \bar{\psi}, \bar{\eta}), z(\varphi_*, \bar{\psi}, \bar{\eta})) \in ABB_*A_*$$

to the point  $(x(\varphi, \bar{\psi}, \bar{\eta}), y(\varphi, \bar{\psi}, \bar{\eta}), z(\varphi, \bar{\psi}, \bar{\eta})) \in G_z$  along the corresponding line of flow (as crossing some two surfaces  $\psi(x, y, z) = \bar{\psi}$ ,  $0 \leq \bar{\psi} \leq Q_*$ ,  $\eta(x, y, z) = \bar{\eta}$ ,  $0 \leq \bar{\eta} \leq Q^*$ ),  $f^{-1}$  is the function inverse to f with respect to the variable  $\varphi$  (we should note that such function exists as  $v^2(\varphi, \psi, \eta)$  is continuously differentiable, limited, positive certain function).

Functions  $\Pi_{i,j}(\xi,\psi,\eta,t)$ ,  $P_j(\xi,\psi,\eta,t)$   $\varphi = \bar{\varphi}^*$ ,  $(j=\overline{0,2})$ ,  $\bar{\Pi}_{i,j}(\bar{\xi},\psi,\eta,t)$ ,  $\bar{P}_j(\bar{\xi},\psi,\eta,t)$ ,  $(j=\overline{0,2})$ ,  $\tilde{\Pi}_{i,j}(\varphi,\tilde{\psi},\eta,t)$ ,  $\bar{\Pi}_{i,j}(\varphi,\tilde{\psi},\eta,t)$ ,  $\bar{\Pi}_{i,j}(\varphi,\psi,\tilde{\tilde{\eta}},t)$ ,  $\bar{\Pi}_{i,j}(\varphi,\psi,\tilde{\eta},t)$  and  $\tilde{P}_j(\varphi,\tilde{\psi},\eta,t)$ ,  $\bar{P}_j(\varphi,\tilde{\psi},\eta,t)$ ,  $\tilde{P}_j(\varphi,\psi,\tilde{\eta},t)$ ,  $(j=\overline{0,3})$  are determined following [9]. The estimation of remainder members is conducted following [10].

## 4. Results of numerical calculations

We represent results of numerical experiment for filter bounded with the following surfaces:

$$f_1(x, y, z) = z - 1.25,$$

$$f_2(x, y, z) = (z - 2.5466434)^2 + y^2 + x^2 - 0.1187841,$$

$$f_3(x, y, z) = (z - 1.25)^2 + (y - 3.8471044)^2 + x^2 - 16.3627124,$$

$$f_4(x, y, z) = (z - 1.25)^2 + x^2 + (y + 3.8471044)^2 + x^2 - 16.3627124,$$

$$f_5(x, y, z) = f_6(x, y, z) = [z(z - 2.5) + y^2 + x^2]^2 + 6.25y^2 - 36.4276695x^2.$$

Such filter is characterized by a considerable spatialness of filing up, "monotony of narrowing" in direction from the inlet to the outlet of filter (a choice of such form is explained by practice), and mutual orthogonality of verges along edges and at angular points (it is substantial for simplification of procedure of construction of spatial conformal mapping). On the basis of [10], a calculation of a dynamic net is constructed in  $G_Z$ ,

$$\varphi(x,y,z) = \bar{\varphi}_i \stackrel{\text{df}}{=} \varphi_* + [(\varphi^* - \varphi_*)i]/n, \quad i = \overline{0,n},$$

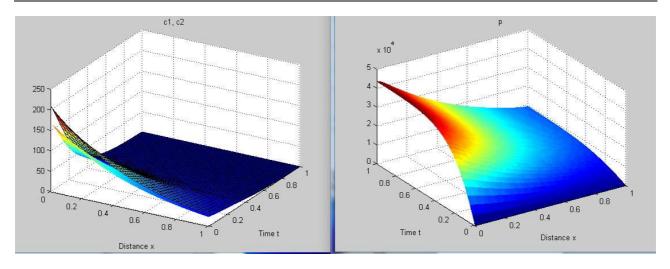
$$\psi(x,y,z) = \bar{\psi}_j \stackrel{\text{df}}{=} (Q_*j)/m, \quad j = \overline{0,m},$$

$$\eta(x,y,z) = \bar{\eta}_k \stackrel{\text{df}}{=} (Q^*k)/l, \quad k = \overline{0,l}$$

for  $\varphi_* = 0$ ,  $\varphi^* = 8000$ , k = 1, n = 30, m = 16, l = 16 (parameters of n, m and l are chosen from the condition of most similarity of the built net to cube), the lauter expense of Q is found = 0.651, the values of filtration rate |v| are calculated. Thus the misclosures of the expected constructions do not exceed 0.001.

In Figure 3, the distribution of concentrations  $c_1$ ,  $c_2$ , and density  $\rho$  is shown along the lines of flow for  $L=1~m,~\beta_i=0.3~{\rm m^2/s},~\alpha_0=0.0056~{\rm m^2/s},~\sigma_0=0.5,~\varepsilon=0.001,~k=1;~c_{1,0}^0(\varphi,\psi,\eta)=0.017\exp\left(-\varphi^2\right),~c_{2,0}^0(\varphi,\psi,\eta)=0.021\exp\left(-\varphi^2\right),~c_{1}^*(\psi,\eta,t)=0.017,~c_{2}^*(\psi,\eta,t)=0.021,~\rho_0^0(\varphi,\psi,\eta)=0.$ 

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**Fig. 1.** Spatial distributions of concentrations  $c_1, c_2,$  and density  $\rho$ 

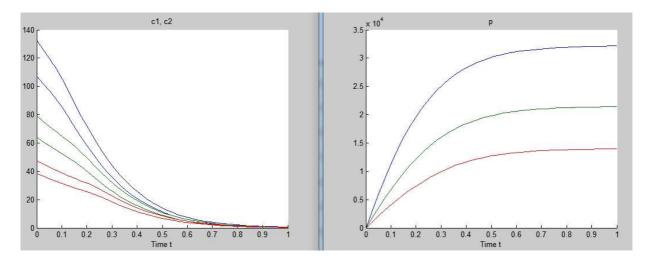


Fig. 2. 2D distributions of concentrations  $c_1$ ,  $c_2$ , and density  $\rho$  during the 10-hour time

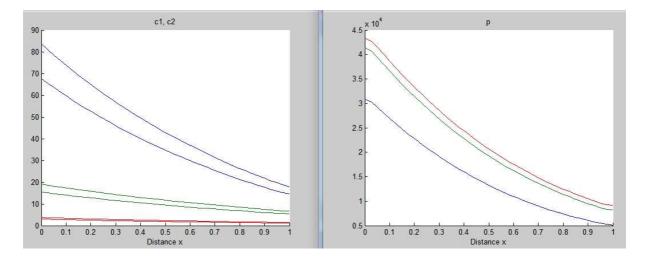


Fig. 3. 2D distributions of concentrations  $c_1,\ c_2,$  and density  $\rho$ 

#### 5. Conclusions

The solution of corresponding nonlinear inverse problem concerning the model that describes the process of multi component decontamination of liquid through filtration in a spatial filter gives us an opportunity to substantially approach numerical calculation to the experimental data (in comparison with the classic phenomenological models), more exactly, to predict and calculate efficiency of the of process of sediment impurities of the different technological water-dispersible systems. The modeling of processes of filtration under the conditions of incomplete data and automation of corresponding processes are of prospect.

[1] Elimelech M. Predicting collision efficiencies of colloidal particles in porous media. Water Research. **26(1)**, 1 (1992)

- [2] Elimelech M. Particle deposition on ideal collectors from dilute flowing suspensions: Mathematical formulation, numerical solution and simulations. Separations Technology. 4, 186 (1994).
- [3] Jegatheesan V. Effect of surface chemistry in the transient stages of deep bed filtration. Ph Dissertation. University of Technology Sydney. (1999).
- [4] Johnson P., Elimelech M. Dynamics of colloid deposition in porous media: Blocking based on random sequential adsorption. Langmuir. **11(3)**, 801 (1995).
- [5] Ison C. R., Ives K. J. Removal mechanisms in deep bed filtration. Che. Engng. Sci. 24, 717 (1969).
- [6] Ives K. J. Rapid filtration. Water Research. 4(3), 201 (1970).
- [7] Petosa A. R., Jaisi D. P., Quevedo I. R., Elimelech M., Tufenkji N. Aggregation and Deposition of Engineered Nanomaterials in Aquatic Environments: Role of Physicochemical Interactions. Environmental Science Technology. 44, 6532 (2010).
- [8] Chaplia Ye. Ya., Chernukha O. Yu. Mathematical modeling of diffusion processes in accidental and regular structures. Naukova dumka. (2009).
- [9] Bomba A. Ya., Baranovskiy S. V., Prisyazhnyk I. M. Nonlinear singularly perturbed problem of "convection diffusion". Rivne: NUWM. (2008).
- [10] Bomba A. Ya., Gavriluk V. I., Safonyk A. P., Fursachyk O. A. Nonlinear filtering problem of the type "diffusion-filtration-mass transfer" under conditions of incomplete data. Monograph. Rivne: NUWM. (2011).
- [11] Ivanchov N. I. On the definition of the time-dependent leading coefficient in a parabolic equation. Sib. mat. journal. **39(3)**, 539 (1998).
- [12] Kabanihin S. I. Inverse and incorrect problems. Novosibirsk: Siberian scientific publishing (2009).
- [13] Mints D. M. Theoretical bases of water treatment technology. M.: Stroyizdat (1964).
- [14] Sergienko I. V., Deineka V. S. Solutions of combined inverse problems for parabolic multi-component distributed systems. Cybernetics and Systems Analysis. 5, 48 (2007).
- [15] Sergienko I. V., Deineka V. S. Identification by gradient methods of the diffusion problems parameters in nanoporous medium. Problems of control and Informatics. 6, 5 (2010).

# Ідентифікація масообмінного коефіцієнта в просторовій задачі фільтрування

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Розглядається задача моделювання процесу очищення рідин від багатокомпонентного забруднення просторовим фільтром, яка враховує зворотний вплив визначальних факторів (концентрації забруднення рідини та осаду) на характеристики середовища (коефіцієнт пористості, дифузії) і надає можливість визначення малого масообмінного коефіцієнта за умов домінування конвективних складових над дифузійними. Запропоновано алгоритм розв'язку відповідної нелінійної оберненої сингулярно збуреної задачі типу «конвекція-дифузія-масообмін».

**Ключові слова:** багатокомпонентність, обернена задача, ідентифікація, умова перевизначення, асимптотичний розв'язок, збурення

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