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HIGH-PERFORMANCE METHODS FOR MODELING AND IDENTIFICATION OF TWO-LEVEL FILTRATION TRANSPORT IN A HETEROGENEOUS MEDIA OF NANOPOROUS PARTICLES

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Abstract. *The paper presents formulations and mathematically justified solutions of nonlinear and linearized models of the «filtration-consolidation» type in heterogeneous multicomponent media saturated with nanoporous particle filtrate, described by boundary value problems for systems of integro-differential equations of the second order. Proposed formulations consider equilibrium mechanisms, the system of multi-interface interactions, and a two-level transport system micro- and nanopores of particles and interparticle space.*

The direct and conjugate problems of parametric identification has been defined, the solutions were substantiated and obtained, and analytical expressions of the gradients of functionals were obtained to restore the studied identification parameters.

Key words: *Two-level filtration, mass transfer, nanoporous particles, integral transformations, high-performance computing, parametric identification.*

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1. INTRODUCTION

Mass transfer of the «filtration-consolidation» type in the medium of filtrate-saturated particles of a microporous structure (solid-liquid filtration-consolidation) is critical technological operation in the processes of liquids extraction from various biological materials and food, chemical industry, pharmacology and other industries. The structure of moisture-rich micro- and nanoporous media is a branched system of moisture-saturated particles, cells, intercellular cavities, micro- and nanopores through which mass transfer is carried out [1, 2].

Mass transfer of the «filtration-consolidation» type is based on the provisions of the theory of filtration consolidation of porous media [3–6]. At the same time, in the classical theory, which is valid for incompressible media, the skeletons of the porous mass are mainly considered to be linearly deformable or deformable in separate (so-called fine-grained) zones of defined gradients. This assumptions do not justify themselves for medias of microporous particles saturated with leachate that are subject to compression.

A factor that needs to be highlighted is that during such transport in a preformed layer of thin saturated particles of a compressible microporous structure, internal and external pressure gradients respectively arise in the particles and in the interparticle space causing leachate outflows from the layer (skeleton) and particles. At the same time, the internal flows of the filtrate directed from the middle of the micropores of the particles to particle surfaces. After that, intermediate flows directed from the outer surfaces of the particles into the macropores of the interparticle space. Macropores of the intraparticle space has external outflows of filtrate to the outside of the layer. Such a phenomenological model in a linear formulation is considered in [7].

We consider a mathematical model of two-level transport «filtration-consolidation» in the system «interparticle space – microporous particles» in nonlinear and linear settings in a heterogeneous multicomponent medium, which takes into account, along with the flow of filtrate in the skeleton, internal flows of filtrate from particles at the micro level. Additionally, model consider the influence of the transit flow of liquid between micropores intraparticle spaces and macropores interparticle spaces. This model based on the relevant mass balance equations in the intraparticle space, including the intra- and intercellular space, and the interparticle space. According to this model, the flow of liquid from micro- and nanopores intraparticle spaces is considered to be insignificant compared to the flow from particles to the outside - into interparticle macropores and the flow of extraparticle spaces to the outside of the layer of the filtration medium. In addition, the considered model includes the assumption of pseudo static flow between intraparticle spaces and interparticle spaces, that is, the flow intensity from the middle of the particle to the outside is directly proportional to the pressure difference inside and outside the particle.

2. MATHEMATICAL MODEL

A mathematical model of two-level transport «filtration-consolidation» in the system «interparticle space – microporous particles» defined for a heterogeneous nanoporous medium that consists of a limited number (n) layers. Such of thin nanoporous layers are perpendicular to the direction of transport (Fig. 1). The model takes into account the interaction of the system of multi-interface interactions, caused by the interface conditions between heterogeneous nanoporous layers of the medium, along with the «particle-media» interaction. Additionally to the two spaces mentioned before like intraparticle space (space of micropores of particles) and interparticle spaces (the space of macropores), here took into account the segment spaces (the space of a separate segment of a heterogeneous environment). Mass transfer in a separate segment is considered in the system of interaction of all other elements of the system.

In the nonlinear formulation of the model, the system of consolidation equations for the heterogeneous region $D=\left\{(t,x,z): t>0,\ 0<r<R,\ z\in\bigcup_{i=1}^{n+1}(l_{k-1},l_k);0\le l_0<l_{n+1}\equiv l\right\}$ will have the form [8]:

$$\frac{\partial}{\partial t}p_{1_k}(t,z)=G_{1_k}(p_{1_1})\frac{\partial}{\partial z}\left(\frac{1}{\mu r_{1k}(p_{1_k})}\frac{\partial}{\partial z}p_{1_k}(t,z)\right)+\beta_2\frac{1}{R}\frac{\partial}{\partial t}\int_0^R p_{2_k}(t,x,z)dx \tag{1}$$

$$\frac{\partial}{\partial t}p_{2_k}(t,z)=G_{2_k}(p_{2_k})\frac{\partial}{\partial z}\left(\frac{1}{\mu r_{2_k}(p_{2_k})}\frac{\partial}{\partial z}p_{2_k}(t,z)\right),\ k=\overline{1,n+1}. \tag{2}$$

Here: $G_{i_k},\frac{1}{\mu_k r_{i_k}}r_{i_k};i=\overline{1,2};\ k=\overline{1,n+1}$ represents the compressibility modules and filtration coefficients for the interparticle space and the micropores space of particles for the k-th layer of the medium.

The initial conditions:

$$p_{1_k}(t,z)_{t=0}=p_{E_k}(z),\qquad p_{2_k}(t,x,z)_{t=0}=p_{E2_k}(x,z) \tag{3}$$

boundary conditions and a interface conditions between segments of a heterogeneous medium) by the variable z

$$\begin{aligned} &p_{1_k}(t,z)\big|_{z=0}=p_{st_k}(t); &&\frac{\partial}{\partial z}p_{1_k}(t,z)\big|_{z=l}=0\\ &\frac{\partial}{\partial x}p_{2_k}(t,R,z)=0; &&p_{2_k}(t,x,z)_{x=R}=p_{1_k}(t,z). \end{aligned} \tag{4}$$

$$\left[p_{1_k}(t,z) - p_{1_{k+1}}(t,z) \right]_{z=\xi_k} = 0;$$
$$\frac{\partial}{\partial z}\left[p_{1_k}(t,z) - \zeta_k p_{1_{k+1}}(t,z) \right]_{z=\xi_k} = 0;\ k=\overline{1,n}; \qquad (5)$$

The linearization scheme based on [9] is used to linearize the consolidation equations of the model (1)–(5).

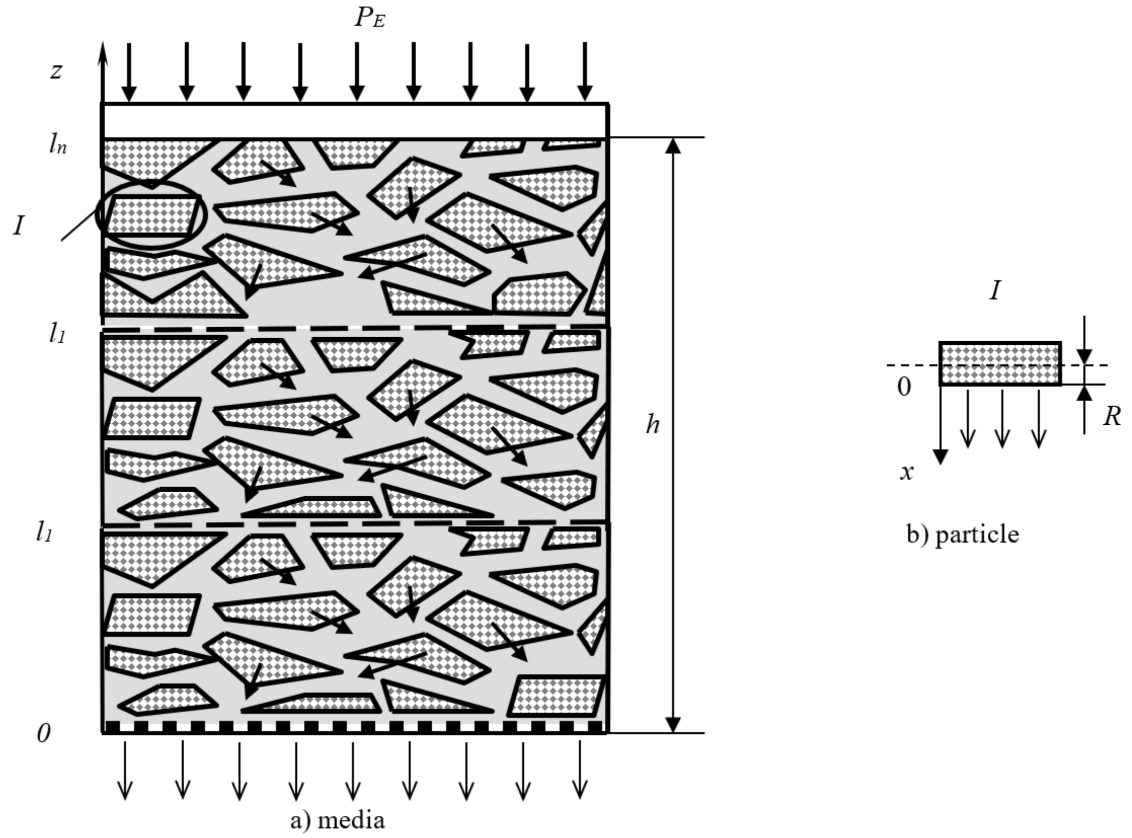


Figure 1. Mass transfer in a two-level pore system for a heterogeneous medium

The direct problem formulation. Let us consider the linearized model of «filtration-consolidation» transport in a heterogeneous media of moisture-saturated microporous particles as the system of boundary problems for partial differential equations: to build a solution of consolidation equation for one layer of nanoporous medium in the domain

$$\frac{\partial}{\partial t}\begin{bmatrix} P_{1_1}(t,z) \\ P_{1_2}(t,z) \\ \dots \\ P_{1_{n+1}}(t,z) \end{bmatrix} = \frac{\partial}{\partial z}\left(\begin{bmatrix} b_{1_1} & 0 & \dots & 0 \\ 0 & b_{1_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & b_{1n+1} \end{bmatrix} \frac{\partial}{\partial z}\begin{bmatrix} P_{1_1}(t,z) \\ P_{1_2}(t,z) \\ \dots \\ P_{1_{n+1}}(t,z) \end{bmatrix} \right) + \beta_{2_k}\frac{1}{R}\frac{\partial}{\partial t}\int_0^R \begin{bmatrix} P_{2_1}(t,x,z) \\ P_{2_2}(t,x,z) \\ \dots \\ P_{2_{n+1}}(t,x,z) \end{bmatrix} dx,$$
$$\frac{\partial}{\partial t}\begin{bmatrix} P_{2_1}(t,z) \\ P_{2_2}(t,z) \\ \dots \\ P_{2_{n+1}}(t,z) \end{bmatrix} = \frac{\partial}{\partial z}\left(\begin{bmatrix} b_{2_1} & 0 & \dots & 0 \\ 0 & b_{2_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & b_{2n+1} \end{bmatrix} \frac{\partial}{\partial z}\begin{bmatrix} P_{2_1}(t,z) \\ P_{2_2}(t,z) \\ \dots \\ P_{2_{n+1}}(t,z) \end{bmatrix} \right), \qquad (6)$$

The initial conditions:

$$P_{1_k}\left(t,z\right)\Big|_{t=0} = P_{E_k}(z);\; P_{2_k}\left(t,x,z\right)\Big|_{t=0} = P_{E2_k}(x,z)\,, \tag{7}$$

The boundary and interface conditions on z

$$P_{1_1}\left(t,z\right)\Big|_{z=0} = 0\,; \qquad \frac{\partial P_{1_{n+1}}}{\partial z}\Big|_{z=l} = 0 \tag{8}$$

$$\begin{aligned}&\left[P_{1_k}(t,z) - P_{1_{k+1}}(t,z)\right]_{z=l_k} = 0;\; k=\overline{1,n}\\ &\frac{\partial}{\partial z}\left[P_{1_k}(t,z) - \zeta_k P_{1_{k+1}}(t,z)\right]_{z=l_k} = 0;\end{aligned}\;; \tag{9}$$

The boundary conditions on x

$$\frac{\partial P_{2_k}}{\partial x}\Big|_{x=0} = 0\,; \qquad P_{2_k}\Big|_{x=R} = P_{1_k}\left(t,z\right). \tag{10}$$

Here P_{1_k}, P_{2_k} – pressure distributions in interparticle spaces and intraparticle space for k -th layer of heterogeneous dispersed medium; $\zeta_k = \dfrac{r_k}{r_{k+1}}$.

Considering that the consolidation factors b_{1_m}, b_{2_m} problems (6)–(10) are unknown and that solution traces for m-th segment are known ($m=\overline{1,n+1}$):

$$P_{1m}\left(t,z\right)\Big|_{\gamma_m} = f_m\left(t,z\right)\Big|_{\gamma_m},\; \bar{P}_{2m}\left(t,z\right)\Big|_{\gamma_m} = g_m\left(t,z\right), \tag{11}$$

$\bar{P}_{2m}\left(t,R/2,z\right) = \dfrac{1}{R}\int_0^R P_{2m}\left(t,r,z\right)rdr$ is average pressure in the particles concentrated in a location $r=R/2$ for m-th layer of the heterogeneous medium, $m=\overline{1,n+1}$.

According to [10], obtained on the basis of

The initial-boundary problem of filtration consolidation (6)–(10) are the similar to the problem of successive thin filtration microporous layers of particles [10] with corresponding conditions:

- first n segments, $k=\overline{1,n}$

$$P_{1_k}\left(t,z\right)\Big|_{l_{k-1}} = P_{1l_{k-1}},\; P_{1_k}\left(t,z\right)\Big|_{l_k} = P_{1l_k},\; k=\overline{1,n+1} \tag{12}$$

- last n+1 segments

$$P_{1_n}\left(t,z\right)\Big|_{l_n} = P_{1l_n},\; \frac{\partial}{\partial z}P_{1_{n+1}}\left(t,z\right)\Big|_{l_{n+1}} = 0, \tag{13}$$

and consists in finding functions $b_{1_m}\in D$, $b_{2_m}\in D$ in domain $D=\left\{v\left(t,z\right):\; v\big|_{\Omega_{m_T}} \in C\left(\Omega_{m_T}\right),\; v>0,\; m=\overline{1,n+1}\;\right\}$.

The discrepancy function that determines the deviation of the desired solution from traces of the solution obtained empirically on the surface of γ_m [10]:

$$J\ (b_1,b_2)=\frac{1}{2}\int_0^T\left(\left\|P_{1_m}(\tau,z,b_1,b_2)-f_m\right\|^2_{L_2(\gamma_m)}+\left\|\bar{P}_{2_m}(\tau,R/2,b_1,b_2)-g_{sm}\right\|^2_{L_2(\gamma_m)}\right)d\tau, \qquad (14)$$

$$\|\varphi\|^2_{L_2(\gamma_m)}=\int_{\gamma_m}\varphi^2 d\gamma \qquad\qquad \|\varphi\|_{L_2(\gamma_m)}=\left|\varphi(t,z)\right|_{z=\gamma_m}.$$

Analytical solution of the model. Let apply the finite integral Fourier transform [11] to equation (6) with conditions (8). As the result we obtain

$$P_{2_k}(t,x,z)=P_{E_k}(z)\frac{2}{R}\sum_{m=0}^{\infty}\frac{(-1)^m}{\eta_m}e^{-b_{2_k}\eta_m^2 t}\cos\eta_m x+\frac{2}{R}\sum_{m=0}^{\infty}(-1)^m b_{2_k}\eta_m\int_0^t e^{-b_{2_k}\eta_m^2(t-\tau)}P_{1_k}(\tau,z)d\tau\cos\eta_m x, \qquad (15)$$

$$\frac{1}{R}\int_0^R P_{2_k}(t,x,z)dx=P_{E_k}(z)\frac{2}{R^2}\sum_{m=0}^{\infty}\frac{1}{\eta_m^2}e^{-b_{2_k}\eta_m^2 t}+\frac{2}{R^2}b_{2_k}\sum_{m=0}^{\infty}\int_0^t e^{-b_{2_k}\eta_m^2(t-\tau)}P_{1_k}(\tau,z)d\tau\cdot \qquad (16)$$

where $\vartheta(x,\eta_m)=\cos\eta_m x$, $\eta_m=\frac{2m+1}{2R}\pi,\quad m=\overline{0,\infty}$ are spectral functions and spectral values of integral transformation.

After that, applying the integral Laplace transform [12] to the problems (6)–(9) and taking into account (15), (16) leads to

$$b_{1_k}\frac{d^2P^*_{1_k}(s,z)}{dz^2}-s\left(1+\frac{\beta_2 2}{R^2}\sum_{m=0}^{\infty}\frac{1}{\frac{s}{b_{2_k}}+\eta_m^2}\right)P^*_{1_k}(s,z)=$$
$$=-\left((1+\beta_2)-s\beta_2\frac{2}{b_{2_k}R_2}\sum_{m=0}^{\infty}\frac{1}{\eta_m^2\left(\frac{s}{b_{2_k}}+\eta_m^2\right)}\right)P_{E_k}(z), \qquad (17)$$

$$P^*_{1_1}\big|_{z=0}=0\ ; \qquad\qquad \frac{dP^*_{n+1}}{dz}\Big|_{z=l}=0\cdot \qquad (18)$$

$$\left[P^*_{1k}(s,z)-P^*_{1k+1}(t,z)\right]_{z=l_k}=0;\ \frac{\partial}{\partial z}\left[P^*_{1k}(s,z)-\zeta_k P^*_{1k+1}(s,z)\right]_{z=l_k}=0;k=\overline{1,n}. \qquad (19)$$

And applying integral Fourier transform for an inhomogeneous medium [12] to the problem (17)–(19) gives the equation

$$\left[\lambda_n^2+s\left(1-\beta_2\frac{2}{R^2}\sum_{m=0}^{\infty}\frac{1}{\frac{s}{b_{2_1}}+\eta_m^2}\right)\right]P^*_{1,n}(s)=\left(1-\beta_2\left(1-\frac{2}{R^2}\sum_{m=0}^{\infty}\frac{\frac{s}{b_{2_1}}}{\eta_m^2\left(\frac{s}{b_{2_1}}+\eta_m^2\right)}\right)\right)P_{E_n}\cdot \qquad (20)$$

In result of transformations

$$P_{1,n}^{*}(s)=P_{E_n}\frac{1}{\left[s+\lambda_n^2-\beta_2\frac{\sqrt{s}\sqrt{b_{2_1}}}{R}th\sqrt{\frac{s}{b_{2_1}}}R\right]}\left[1-\beta_2\frac{sh\sqrt{\frac{s}{b_{2_1}}}R}{\sqrt{\frac{s}{b_{2_1}}}Rch\sqrt{\frac{s}{b_{2_1}}}R}\right]. \qquad (21)$$

In equations (21) back to originals [12] gives

$$P_{1,n}(t)=P_{E_n}L^{-1}\left[\frac{1}{s+\lambda_n^2-\beta_2\frac{\sqrt{s}\sqrt{b_{2_1}}}{R}th\sqrt{\frac{s}{b_{2_1}}}R}\right]-\beta_2L^{-1}\left[\frac{1}{s+\lambda_n^2-\beta_2\frac{\sqrt{s}\sqrt{b_{2_1}}}{R}th\sqrt{\frac{s}{b_{2_1}}}R}\right]*L^{-1}\left[\frac{sh\sqrt{\frac{s}{b_{2_1}}}R}{\sqrt{\frac{s}{b_{2_1}}}R\cdot ch\sqrt{\frac{s}{b_{2_1}}}R}\right], \qquad (22)$$

where * represents two functions convolution.

Finally, we get back to original, based on the Heaviside expansion theorem, [12, 14]

$$P_{1,n}(t)=P_{E_n}\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2 t}}{1-\frac{\beta_2}{2}\left(\frac{\sqrt{b_{2_1}}}{\nu_{jn}R}tg\frac{\nu_{jn}R}{\sqrt{b_{2_1}}}+\frac{1}{\cos^2\frac{\nu_{jn}R}{\sqrt{b_{2_1}}}}\right)}\left[1-\beta_2\frac{2b_{2_1}}{R^2}\sum_{i=0}^{\infty}\int_0^t e^{-\left(b_{2_1}\mu_i^2-\nu_{jn}^2\right)\tau}d\tau\right]. \qquad (23)$$

Here ν_{jm}, $j=\overline{1,\infty}, n=\overline{0,\infty}$ is set of transcendental equation roots:

$$\nu^2-\lambda_n^2-\beta_2\cdot\nu\frac{\sqrt{b_{2_1}}}{R}tg\frac{\nu}{\sqrt{b_{2_1}}}R=0, \qquad \mu_i=\frac{(2i+1)\pi}{2R},\quad \mathrm{i}=\overline{1,\infty}$$

The transition to the original by variable z gives an expression for vector function $P_{1_k}(t,z)$. This function describe the pressure distribution in the interparticle spaces [11, 13, 15]

$$P_{1_k}(t,z)=\sum_{k_1=1}^{n+1}\int_{l_{k_1-1}}^{l_{k_1}}\mathrm{H}_{1_{k,k_1}}(t,z,\xi)P_{E_{k_1}}(\xi)d\xi, \qquad (24)$$

Where: $\left[\mathrm{H}_{1_{k,k_1}}(t,z,\xi)\right]$, $k,k_1=\overline{1,n+1}$ are elements of influence function's matrix. Such elements defined by expression:

$$\mathrm{H}_{1_{k,k_1}}(t,z,\xi)=\sum_{n=0}^{\infty}\sum_{j=1}^{\infty}\frac{e^{-b_{2_1}\nu_{jn}^2 t}}{1-\frac{\beta_2}{2}\left(\frac{\sqrt{b_2}}{\nu_{jn}R}tg\frac{\nu_{jn}R}{\sqrt{b_2}}+\frac{1}{\cos^2\frac{\nu_{jn}R}{\sqrt{b_2}}}\right)}\left(1-\beta_2\frac{2}{R^2}\sum_{i=0}^{\infty}\frac{1-e^{-\left(b_{2_1}\mu_i^2-b_{2_1}\nu_{jn}^2\right)t}}{1-\frac{\nu_{jn}^2}{b_{2_1}\mu_i^2}}\frac{1}{\mu_i^2}\right).$$

After substitution equation $P_1(t,z)$ in (15), we calculate components of the vector function $P_{2_k}(t,x,z)$. Such function define pressure distribution in micropores intraparticle spaces

$$P_{2_k}(t,x,z)=\frac{2}{R}\sum_{m=0}^{\infty}\left[\begin{array}{l}P_{E_k}(z)e^{-b_{2_k}\eta_m^2 t}+\\+\sum_{k=1}^{n+1}\int_{l_{k_1-1}}^{l_{k_1}}\text{H}_{2_{k,k_1}}(t,z,\xi)P_{E_{k_1}}(\xi)d\xi\end{array}\right]\frac{(-1)^m\cos\eta_m x}{\eta_m}, \quad (25)$$

where: $\left[\text{H}_{1_{k,k_1}}(t,z,\xi)\right]$, $k,k_1=\overline{1,n+1}$ are elements of the influence function's matrix.

$$\text{H}_{2_{k,k_1}}(t,z,\xi)=\sum_{j=1}^{\infty}\frac{V_{k_1}(\xi,\lambda_j)V_k(z,\lambda_j)}{\left\|V(z,\lambda_j)\right\|^2}\sum_{n=0}^{\infty}\frac{\text{E}_k(t,\nu_{jn},\eta_m)}{1-\frac{\beta_2}{2}\left(\frac{\sqrt{b_2}}{\nu_{jn}R}tg\frac{\nu_{jn}R}{\sqrt{b_2}}+\frac{1}{\cos^2\frac{\nu_{jn}R}{\sqrt{b_2}}}\right)}.$$

$$\text{E}_k(t,\nu_{jn},\eta_m)=\left(\begin{array}{l}\frac{e^{-b_{2_1}\nu_{jn}^2 t}-e^{-b_{2_k}\eta_m^2 t}}{1-\frac{b_{2_1}\nu_{jn}^2}{b_{2_k}\eta_m^2}}-\\-\beta_2\frac{2}{R^2}\sum_{i=0}^{\infty}\frac{\frac{e^{-b_{2_1}\nu_{jn}^2 t}-e^{-b_{2_k}\eta_m^2 t}}{1-\frac{b_{2_1}\nu_{jn}^2}{b_{2_k}\eta_m^2}}-\frac{e^{-b_{2_1}\mu_i^2 t}-e^{-b_{2_k}\eta_m^2 t}}{1-\frac{b_{2_1}\mu_i^2}{b_{2_k}\eta_m^2}}}{1-\frac{\nu_{jn}^2}{b_{2_1}\mu_i^2}}\frac{1}{\mu_i^2}\end{array}\right).$$

3. NUMERICAL MODELING AND DISCUSSION

The numerical modeling based on the analytical solution of the described model (6)–(9) was done with specialized high-performance computing software. We have modeled the pressure distributions in the macropores of the interparticle space $P_1(t,z)$ and pressure distributions in intraparticle space micropores $P_2(t,x,z)$ under different initial process conditions. For the modeling process, the results of which are given below, the following characteristics of the physical process were used: $h=0.01$, $R=0.008$, $\beta_2=0.05$, $G_{10}/r_{10}=2\cdot 10^{-10}$, $G_{20}/r_{20}=1\cdot 10^{-9}$, $\mu=10^{-3}$, $\alpha=0.0002$, $P_e=1$. Pressure distribution curves are presented as functions of time and dimensionless geometric coordinates $X=x/R$ and $Z=z/h$.

Fig. 2 shows the pressure changes in macropores $P_1(t,z)$ during process time t for different coordinate of media layer Z. The pressure $P_1(t,z)$ decreases exponentially over time. and in comparison with the linear model, clearly observable nonlinearities in the pressure profile associated with the dependence of the ratio b_{1_k}/b_{2_k} of the consolidation coefficients on the pressure for every layer.

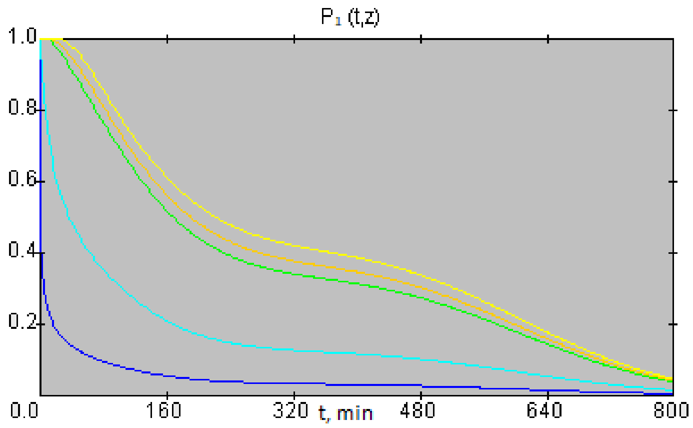


Figure 2. Pressure profile evolution in macropores at time for various locations at a heterogeneous media Z=1.0 (yellow), Z=0.7 (orange), Z=0.6 (green), Z=0.2 (cyan), Z=0.05 (blue)

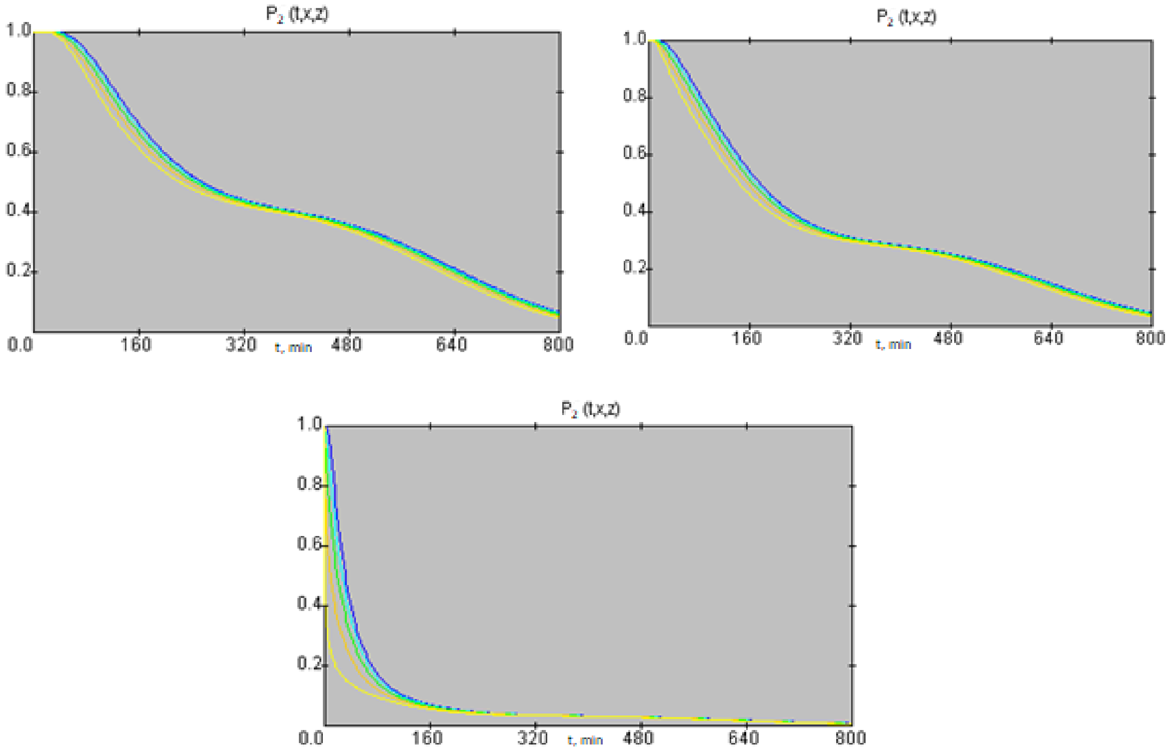
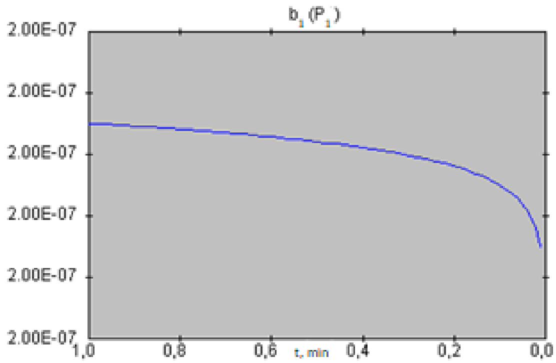


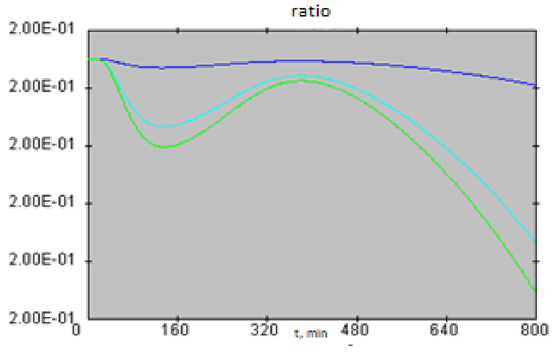
Figure 3. Pressure profile evolution in micropores at time for various position of the particle in the medium: a) Z=1; b) Z=0.5; c) Z=0.05; X=1 (yellow), X=0.8 (orange), X=0.6(green), X=0.4(cyan), X=0.05(blue)

Fig. 3 shows the profiles of pressure in micropores of intraparticle spaces $P_2(t, X, Z)$ changes in time for various particle thickness coordinate X. On the graph, curve Z=1 corresponds to the position of the particle on the surface of the layer, Z =0.5 corresponds to the position of the particle in the middle of the layer and Z =0 corresponds to the position right next to the filtration membrane. As for the pressure in the interparticle space, we can observe a general similarity with the linear models and well-defined non-linearity in the pressure profile.

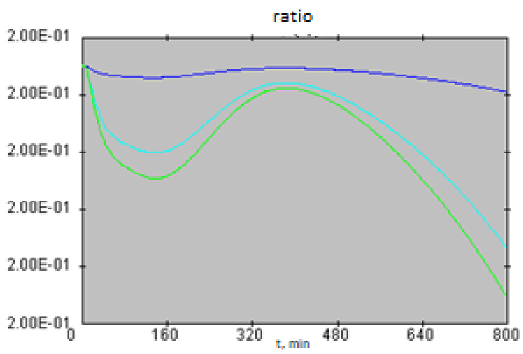
The fig.4 shows the dependence of nonlinear consolidation coefficient on the pressure value. The plots (b), (c) and (d) represents the dynamic changes in the ratio $\frac{b_1}{b_2}\left(\frac{P_1}{P_2}\right)^2$ of nonlinear consolidation coefficients in interparticle and intraparticle spaces over time for various positions in a dispersed medium.



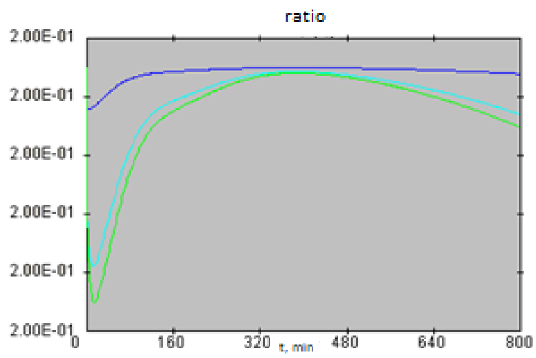
a)



b)



c)



d)

Figure 4. Consolidation coefficients a) - Dependence of the nonlinear consolidation coefficient on the pressure value, b), c), d) - Ratio of nonlinear consolidation coefficients in the interparticle and intraparticle spaces b) Z=1, c) Z=0.5, d) Z =0.05, X=0.95 (blue), X=0.5(cyan), X=0.05 (green)

4. CONCLUSIONS

The formulations and solutions of a nonlinear «filtration-consolidation» type model are proposed. The model described by mixed boundary problems for systems of integro-differential equations of the second order in heterogeneous multilayered media of nanoporous particles, and considers the mechanisms of equilibrium, the system of multi-interface interactions, the two-level transfer of the system micro- and nanopores of particles (micro-level) and interparticle space (macro-level). Such a model allows the study the parameters of filtration consolidation and imprinting of media saturated with filtrate of nanoporous particles.

Moreover, the formulations of direct and conjugate problems for parametric identification for heterogeneous «filtration-consolidation» systems give the opportunity for substantiated and obtained, and analytical expressions of gradients of functionals and to restore the studied identification parameters.

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ВИСОКОЕФЕКТИВНІ МЕТОДИ МОДЕЛЮВАННЯ ТА ІДЕНТИФІКАЦІЇ ДВОРІВНЕВОГО ФІЛЬТРАЦІЙНОГО ТРАНСПОРТУ В НЕОДНОРІДНОМУ СЕРЕДОВИЩІ НАНОПОРИСТИХ ЧАСТИНОК

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Резюме. *Досліджено високоефективні методи моделювання та індентифікації дворівневого фільтраційного транспорту в неоднорідних середовищах нанопористих частинок, при якому в окремо взятому сеґменті масоперенос розглянуто в системі взаємовпливу усіх інших елементів системи: intraparticle spaces – segment interparticle spaces – medium interparticle spaces. Для цього виконано* *фізико-математичну постановку та математично обґрунтовані розв'язки нелінійних та лінеаризованих моделей типу «фільтрація-консолідація» в неоднорідних багатоскладових середовищах, насичених фільтратом нанопористих частинок, що описані крайовими задачами інтегро-диференціальних рівнянь другого порядку, які враховують механізми рівноваги, системи багатоінтерфейсних взаємодій, дворівневого переносу як системи мікро- та нанопористих частинок, так і міжчастинкового простору. Постановку виконано в нелінійній формі та проведено лінеаризацію рівнянь консолідації запропонованої моделі з застосуванням схем лінеаризації. Аналітичні розв'язки моделі являють собою функції тисків в interparticle spaces та intraparticle spaces та побудовані із застосуваванням скінченних інтегральних перетворень Фур'є та Лапласа і теореми про розвинення Гевісайда. Виконано постановки прямих і спряжених задач параметричної ідентифікації для систем типу «фільтрація-консолідація» в неоднорідних середовищах мікропористих частинок, обґрунтовано та отримано їх розв'язки. Проведено числове моделювання з використанням високопродуктивного програмного забезпечення, розробленого на основі побудованих розв'язків математичної моделі та прямих і спряжених задач параметричної ідентифікації. В результаті змодельовано розподіли тисків у макропорах міжчастинкового середовища та розподіли тисків у мікропорах, а також отримано залежності коефіцієнтів консолідації від часу й положення в середовищі та динамічні зміни відношення коефіцієнтів нелінійної консолідації в міжчастинковому та внутрічастинковому просторах у часі для різних положень у дисперсному середовищ. Отримані розподіли тисків представлені як функції часу та безрозмірних геометричних координат. Отримані результати можуть бути використані для дослідження параметрів фільтраційної консолідації та відтиску середовищ насичених фільтратом нанопористих частинок. Отримані аналітичні вирази градієнтів функціоналів можна застосовувати для ідентифікації параметрів внутрішньої кінетики досліджуваних процесів масопереносу.*

Ключові слова: *дворівневий фільтраційний перенос, нанопористі частинки, інтегральні перетворення, операційний метод Гевісайда, параметриична ідентифікація.*

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