Вісник Тернопільського національного технічного університету
https://doi.org/10.33108/visnyk_tntu
Scientific Journal of the Ternopil National Technical University
2022, № 4 (108) https://doi.org/10.33108/visnyk_tntu2022.04
ISSN 2522-4433. Web: ***visnyk.tntu.edu.ua***

UDC 519.6

HIGH-PERFORMANCE INTELLECTUAL INFORMATION TECHNOLOGIES FOR THE STUDY OF FILTRATION SYSTEMS IN DIFFERENT-SIZED NANOPOROUS PARTICLES MEDIA

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Summary. *In the paper, the technologies for the high-performance intellectual nanoporous filtration systems based on the mathematical model of the two-level transport «filtration-consolidation» in the system of nanopores in two intraparticle spaces, which includes two subspaces of different-sized nanoporous particles are developed.*

Key words: *Nanofiltration processes, numerical modeling, parallel computing, science-intensive technologies, different-sized nanoporous particles media.*

https://doi.org/10.33108/visnyk_tntu2022.04.016 *Received 20.12.2022*

Statement of the problem. Complex systems and processes designed in the field of environmental protection, emission reduction, medicine, and liquids or gases filtration require a new high-performance information systems creation for their research based on scientific mathematical models with high-quality physical substantiation of the composition of their elements, connections between them and parameters that determine efficiency their progress and work.

Analysis of the available investigations. The proposed information technology for the study of nanoporous filtration systems is based on the one developed by us phenomenological model of the two-phase and two-level two-level transport «nanofiltration-consolidation» in the «interparticle space – nanoporous particles» system, which takes into account the complex feedback-interaction of the internal flow of adsorbed substance from the nanopores of spherical particles and the mass flow of the substance located in the interparticle space [1, 2].

Formulation of the problem. The nanoporous medium is considered a multi-level porous system with interparticle and intraparticle networks for express fluid flows. We consider nanoporous particles containing a liquid substance consisting of various chemical components. The particles form a nanoporous layer that is subject to one-dimensional compression (Fig. 1). Substance flows interact between all considered spaces. Nanoporous particles are separated by a porous membrane. A layer of particles is considered a two-pore medium. In fig. 1 shows two levels of the considered elementary volume: level 1(a) for the system of macropores in the interparticle space (interparticle space) and level 2 (b and c) for the system of nanopores in intraparticle spaces, which includes two subspaces of particles of different sizes: intraparticle space1 – the space of nanoporous particles with a radius of at least R_1 and intraparticle space 2 – the space of nanoporous particles with a radius of at least R_2 ($R_1 > R_2$).

Mathematical model. The mathematical model of the considered complex system of nanofiltration and nano diffusion in the spaces of different-sized nanoporous particles, taking into account the specified physical factors and feedback interactions, can be described in the form of a system of boundary value problems for partial differential equations for three of the indicated interconnected spaces formed for all spaces (interparticle space and two intraparticle spaces) relative to the liquid phase.

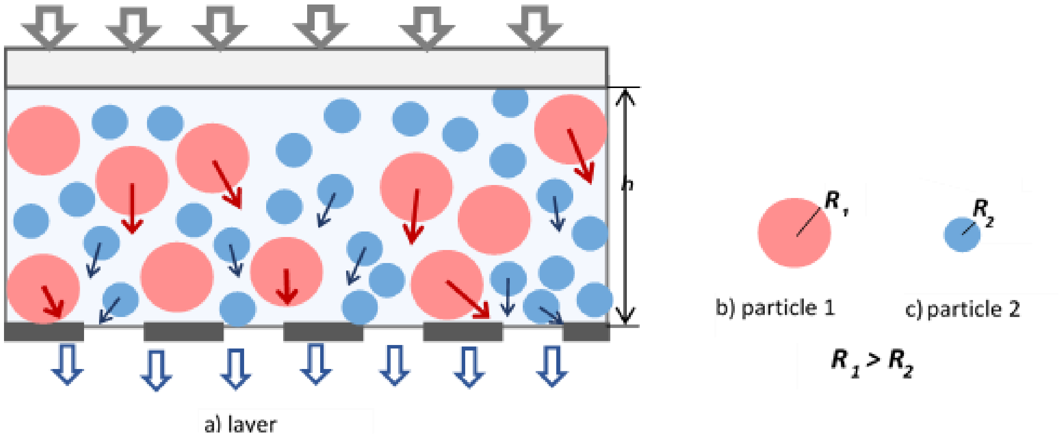

Figure 1. Schematization of flow interactions in a two-level system of nanopores between spaces intraparticle space 1, intraparticle space 2

Problem A (consolidation equation for the interparticle space) consists in finding a limited solution of the consolidation equation for a layer with different-sized nanoporous particles in the domain

$$D_1 = \{(t,z): t>0,\ \ 0<z<h\}:$$

$$\frac{\partial P_1(t,z)}{\partial t} = b_1 \frac{\partial^2 P_1}{\partial z^2} - \beta_1 \frac{\varepsilon}{R_1}\frac{\partial}{\partial t}\int_0^{R_1} P_2(t,x_1,z)dx_1 - \beta_2 \frac{1-\varepsilon}{R_2}\frac{\partial}{\partial t}\int_0^{R_2} P_3(t,x_2,z)dx_2 \qquad (1)$$

with the initial condition:

$$P_1(t,z)\big|_{t=0} = P_E, \qquad (2)$$

the boundary conditions (for variable *z*)

$$P_1(t,z)\big|_{z=0} = 0; \qquad \frac{\partial P_1}{\partial z}\Big|_{z=h} = 0 \qquad \text{(impermeability condition);} \qquad (3)$$

Problems B1, 2 (consolidation equations for particles) to find the limited solutions of the consolidation equations for the nanoporous particles (radius R_i) in the domain

$$D_i = \{(t,x_i,z): t>0,\ \ |x_i|<R_i,\ \ 0<z<h,\ \ i=2,3\}:$$

$$\frac{\partial P_i}{\partial t} = b_i \frac{\partial^2 P_i}{\partial x_j^2},\ \ i=\overline{2,3},\ \ j=\overline{1,2} \qquad (4)$$

with the initial conditions:

$$P_i\big|_{t=0} = P_E(z),\ \ i=\overline{2,3} \qquad (5)$$

the boundary conditions (for radial variable x_j) are:

$$\frac{\partial P_i}{\partial x_j}\Big|_{x_j=0}=0\,;\;\; P_i(t,x_j,z)\big|_{x_j=R_j}=P_1(t,z)\,. \qquad (6)$$

Nomenclature: P_1 – liquid pressure in interparticle space, P_2, P_3 – liquid pressure in intraparticle space 1 and intraparticle space 2 (interior of spherical particles 1 and 2) in accordance, b_1 – is a consolidation coefficient in interparticle space, b_2, b_3 – consolidation coefficients in intraparticle space 1 and intraparticle space 2, $\beta_{1,}$, β_2 – elasticity factor of the particles 1 and 2 in accordance, h – is layer thickness, R_1, R_2 – radius of particles 1 and 2.

Analytical solution. A pressure profile in interparticle spaces and intraparticle spaces 1 and intraparticle spaces 2. The analytical solution to the problem is found using the operational Heaviside's method, Laplace integral, and Fourier integral transformations.

Applying the finite integral Fourier transform (cos) [3, 4]:

$$F_c\left[P_i\left(t,x_j,z\right)\right]=\int_0^{R_j}P_i(t,x_j,z)\vartheta\left(x_j,\eta_{m_j}\right)dx_j=\int_0^{R_j}P_i(t,x_j,z)\cos\eta_{m_j}x_j dx_j\equiv P_{im_j}\left(t,z\right),\; i=\begin{cases}2, & j=1\\ 3, & j=2\end{cases}$$

$$F_c^{-1}\left[P_{im_j}\left(t,z\right)\right]=\sum_{m_j=0}^{\infty}P_{im_j}\left(t,z\right)\frac{\vartheta\left(x_j,\eta_{m_j}\right)}{\left\|\vartheta\left(x_j,\eta_{m_j}\right)\right\|^2}=\frac{2}{R_1}\sum_{m_1=0}^{\infty}P_{im_j}(t,z)\cos\eta_{m_j}x_j\equiv P_i\left(t,x_j,z\right),\; i=\begin{cases}2, & j=1\\ 3, & j=2\end{cases}$$

$$F_c\left[\frac{\partial P_i}{\partial x_j^{\,2}}\right]=\int_0^{R}\frac{\partial^2 P_i}{\partial x_j^{\,2}}\vartheta\left(x_j,\eta_{m_j}\right)dx_j=-\eta_{m_j}^2P_{im_j}(t,z)+\left(-1\right)^{m_j}\eta_{m_j}P_1\left(t,z\right),\; i=\begin{cases}2, & j=1\\ 3, & j=2\end{cases}$$

were $\vartheta\left(x_j,\eta_{m_j}\right)=\cos\eta_{m_j}x_j$, $\eta_{m_j}=\dfrac{2m_j+1}{2R_j}\pi$, $m_j=\overline{0,\infty}$ – are the spectral functions and spectral numbers of integral Fourier transform (cos), we obtain the solutions of the problems B_1, B_2:

$$P_2\left(t,x,z\right)=P_E\left(z\right)\frac{2}{R_1}\sum_{m_1=0}^{\infty}\frac{(-1)^{m_1}}{\eta_{m_1}}e^{-b_2\eta_{m_1}^2t}\cos\eta_{m_1}x+\frac{2}{R_1}\sum_{m_1=0}^{\infty}(-1)^{m_1}b_2\eta_{m_1}\int_0^t e^{-b_2\eta_{m_1}^2\left(t-\tau\right)}P_1\left(\tau,z\right)dz\cos\eta_{m_1}x,\;\;|x|\le R_1$$

$$P_3\left(t,x,z\right)=P_E\left(z\right)\frac{2}{R_2}\sum_{m_2=0}^{\infty}\frac{(-1)^{m_2}}{\eta_{m_2}}e^{-b_3\eta_{m_2}^2t}\cos\eta_{m_2}x+\frac{2}{R_3}\sum_{m_2=0}^{\infty}(-1)^{m_2}b_3\eta_{m_2}\int_0^t e^{-b_3\eta_{m_2}^2\left(t-\tau\right)}P_1\left(\tau,z\right)dz\cos\eta_{m_2}x,\;\;|x|\le R_2 \qquad (7)$$

Substituting the expressions (7) into the consolidation equation (1), after a series of transformations and successive application to the problem (1)–(3) of the integral Laplace transform [3] and the finite integral Fourier transform (sin):

$$F_s\left[P_1^*\left(s,z\right)\right]=\int_0^h P_1^*\left(s,z\right)\cdot V\left(z,\lambda_n\right)dz=\int_0^h P_1^*\left(s,z\right)\cdot\sin\lambda_n z dz=P_{1,n}^*(s)\,,$$

$$F_s^{-1}\left[P_{1,n}^*\left(s\right)\right]=\sum_{n=0}^{\infty}P_{1,n}^*\left(s\right)\frac{V(z,\lambda_n)}{\left\|V(z,\lambda_n)\right\|^2}=\frac{2}{h}\sum_{n=0}^{\infty}P_{1,n}^*\left(s\right)\sin\lambda_n z\equiv P_1^*\left(s,z\right)\,,$$

$$F_s\left[\frac{d^2P_1^*(s)}{dz^2}\right]=-\lambda_n^2P_{1,n}^*(s,z),$$

were $V(z,\lambda_n)=\sin\frac{2n+1}{2h}\pi$ – are the spectral functions and $\lambda_n=\frac{2n+1}{2h}\pi$ – are the spectral numbers of integral Fourier transformation (Sin-Fourier).

Applying the integral operator of the inverse integral Laplace transformation to expression (8) we obtain [5, 6]:

$$\left(\lambda^n+\frac{s}{b_1}\left(1+2\frac{\beta_1\varepsilon}{R_1^2}\sum_{m_1=0}^{\infty}\frac{1}{s/b_2+\eta_{m_1}^2}+2\frac{\beta_2(1-\varepsilon)}{R_2^2}\sum_{m_2=0}^{\infty}\frac{1}{s/b_3+\eta_{m_2}^2}\right)\right)P_{1_n}^*(s)=$$
$$=-\frac{1}{b_1}\left(2\frac{\beta_1\varepsilon}{R_1^2}\sum_{m_1=0}^{\infty}\frac{s/b_2}{s/b_2+\eta_{m_1}^2}+2\frac{\beta_2(1-\varepsilon)}{R_2^2}\sum_{m_2=0}^{\infty}\frac{s/b_3}{s/b_3+\eta_{m_2}^2}\right)\frac{P_E}{\lambda_n}+$$
$$+\left(\frac{1+\beta_1\varepsilon}{b_1}+\frac{1+\beta_2(1-\varepsilon)}{b_1}\right)P_E\,\frac{1}{\lambda_n}$$

Using seris [3, 5]

$$\sum_{m_1=0}^{\infty}\frac{1}{s/b_2+\eta_{m_1}^2}=\frac{R_1}{2}\sqrt{\frac{b_2}{s}}th\left(\sqrt{\frac{s}{b_2}}R_1\right)$$

$$\sum_{m=0}^{\infty}\frac{s}{\eta_m^2\left(s+b_2\eta_m^2\right)}=\sum_{m=0}^{\infty}\left(\frac{1}{\eta_m^2}-\frac{1}{s/b_2+\eta_m^2}\right)=\frac{R_1^2}{2}-\frac{R_1}{2}\sqrt{\frac{b_2}{s}}th\left(\sqrt{\frac{s}{b_2}}R_1\right)$$

as result we obtain

$$P_{1_n}^*(s)=\left(b_1\lambda^n+s+\beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\beta_2(1-\varepsilon)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)\right)^{-1}\cdot$$
$$\cdot\left(2+\frac{\beta_1\varepsilon}{R_1}\sqrt{\frac{b_2}{s}}th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\frac{\beta_2(1-\varepsilon)}{R_2}\sqrt{\frac{b_3}{s}}th\left(\sqrt{\frac{s}{b_3}}R_2\right)\right)P_E\,\frac{1}{\lambda_n} \tag{8}$$

Introducing the notation

$$\phi\left(s,\lambda^n\right)=s+b_1\lambda^n+\beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\beta_2(1-\varepsilon)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)$$

and applying the integral operator of the inverse Laplace transformation, we obtain the formula for making the transition to the original in equation (8):

$$P_{1,n}(t) = P_E \frac{2}{\lambda_n} L^{-1}\left[\frac{1}{\phi\left(s,\lambda^n\right)}\right] + P_E \frac{\beta_1 \varepsilon}{\lambda_n} L^{-1}\left[\frac{1}{\phi\left(s,\lambda^n\right)}\right] * L^{-1}\left[\frac{sh\sqrt{\frac{s}{b_2}}R_1}{\sqrt{\frac{s}{b_2}}R_1 ch\sqrt{\frac{s}{b_2}}R_1}\right] + $$
$$+ P_E \frac{\beta_2(1-\varepsilon)}{\lambda_n} L^{-1}\left[\frac{1}{\phi\left(s,\lambda^n\right)}\right] * L^{-1}\left[\frac{sh\sqrt{\frac{s}{b_3}}R_2}{\sqrt{\frac{s}{b_3}}R_2 ch\sqrt{\frac{s}{b_3}}R_2}\right] \quad (9)$$

where $L^{-1}[...]$ – integral operator of inverse Laplce transformation, " * " – is an operator of convolution of both functions. Now we can consider the next equation:

$$s + b_1\lambda^n + \beta_1\varepsilon \frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right) = 0\,.$$

Replacing $i\sqrt{s} = \nu$ or $s = -\nu^2$, we obtain:

$$\nu^2 - b_1\lambda_n^2 - \beta_1\varepsilon\nu \frac{\sqrt{b_2}}{R_1} tg\left(\frac{\nu R_1}{\sqrt{b_2}}\right) - \beta_2(1-\varepsilon)\nu\frac{\sqrt{b_3}}{R_2} tg\left(\frac{\nu R_2}{\sqrt{b_3}}\right) = 0\,. \quad (10)$$

According to Heviside theorem one can obtain the expression of transfer to original [4]:

$$\cdot L^{-1}\left[\frac{1}{s + b_1\lambda^n + \beta_1\varepsilon \frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)}\right] =$$
$$= \frac{1}{2\pi i}\int\limits_{\gamma} \frac{e^{st}ds}{s + b_1\lambda^n + \beta_1\varepsilon \frac{\sqrt{b_2}}{R_1}\sqrt{s}th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}th\left(\sqrt{\frac{s}{b_3}}R_2\right)} = \quad (11)$$
$$= \sum_{j=0}^{\infty} \left.\frac{e^{st}}{\frac{d}{ds}\left[s + b_1\lambda^n + \beta_1\varepsilon \frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)\right]}\right|_{s=-\nu_{jn}^2},$$

where ν_{jn}, j= $\overline{1,\infty}$; $n = \overline{0,\infty}$ – the roots of transcendental equation (10).

Calculating of the denominator in (11):

$$\frac{d}{ds}\left[s+b_1\lambda^n+\beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)\right]\Bigg|_{s=-\nu_{jn}^2}$$

$$=1+\beta_1\varepsilon\frac{\sqrt{b_2}}{2R_1}\left(\frac{1}{\nu_{jn}}tg\left(\nu_{jn}\frac{R_1}{\sqrt{b_2}}\right)+\frac{R_1}{\sqrt{b_2}}\frac{1}{\cos^2\left(\nu_{jn}\frac{R}{\sqrt{b_2}}\right)}\right)+\beta_2(1-\varepsilon)\frac{\sqrt{b_3}}{2R_2}\left(\frac{1}{\nu_{jn}}tg\left(\nu_{jn}\frac{R_2}{\sqrt{b_3}}\right)+\frac{R_2}{\sqrt{b_3}}\frac{1}{\cos^2\left(\nu_{jn}\frac{R_2}{\sqrt{b_3}}\right)}\right)$$

Then, as result, the expression (11) will have the vie:

$$L^{-1}\left[\frac{1}{s+b_1\lambda^n+\beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)}\right]=\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2t}}{1+\Phi\left(\nu_{jn}\right)}$$

were

$$\Phi\left(\nu_{jn}\right)=1+\beta_1\varepsilon\frac{\sqrt{b_2}}{2R_1}\left(\frac{1}{\nu_{jn}}tg\left(\nu_{jn}\frac{R_1}{\sqrt{b_2}}\right)+\frac{R_1}{\sqrt{b_2}}\frac{1}{\cos^2\left(\nu_{jn}\frac{R}{\sqrt{b_2}}\right)}\right)+$$

$$+\beta_2(1-\varepsilon)\frac{\sqrt{b_3}}{2R_2}\left(\frac{1}{\nu_{jn}}tg\left(\nu_{jn}\frac{R_2}{\sqrt{b_3}}\right)+\frac{R_2}{\sqrt{b_3}}\frac{1}{\cos^2\left(\nu_{jn}\frac{R_2}{\sqrt{b_3}}\right)}\right).$$

We calculate the Laplace originals of expressions:

$$L^{-1}\left[\frac{sh\sqrt{\frac{s}{b_2}}R_1}{\sqrt{\frac{s}{b_2}}R_1\cdot ch\sqrt{\frac{s}{b_2}}R_1}\right]=\sum_{k=0}^{\infty}\frac{i(-1)^k e^{-b_2\eta_k^2t}}{\frac{d}{ds}\left[\sqrt{\frac{s}{b_2}}R_1\cdot ch\sqrt{\frac{s}{b_2}}R_1\right]\Big|_{s=-\eta_k^2}}=-b_2\frac{2}{R_1^2}\sum_{k=0}^{\infty}e^{-b_2\eta_k^2t}\cdot$$

$$L^{-1}\left[\frac{sh\sqrt{\frac{s}{b_3}}R_2}{\sqrt{\frac{s}{b_3}}R_2ch\sqrt{\frac{s}{b_3}}R_2}\right]=\sum_{k=0}^{\infty}\frac{i(-1)^k e^{-b_3\eta_k^2t}}{\frac{d}{ds}\left[\sqrt{\frac{s}{b_3}}R_2ch\sqrt{\frac{s}{b_3}}R_2\right]\Big|_{s=-\eta_k^2}}=-b_3\frac{2}{R_2^2}\sum_{k=0}^{\infty}e^{-b_2\mu_k^2t} \qquad (12)$$

In result of this transforms, we obtain the original of function P_1

$$P_1(t,z)=P_E\frac{2}{h}\sum_{n=0}^{\infty}\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2 t}}{\Phi(\nu_{jn})}\left[1-\beta_1\varepsilon\frac{2}{R_1^2}\sum_{k=0}^{\infty}\frac{1-e^{-b_2\left(\eta_k^2-\frac{\nu_{jn}^2}{b_2}\right)t}}{\left(\eta_k^2-\frac{\nu_{jn}^2}{b_2}\right)}-\beta_2(1-\varepsilon)\frac{2}{R_2^2}\sum_{k=0}^{\infty}\frac{1-e^{-b_3\left(\mu_k^2-\frac{\nu_{jn}^2}{b_3}\right)t}}{\left(\mu_k^2-\frac{\nu_{jn}^2}{b_3}\right)}\right]\frac{\sin\lambda_n z}{\lambda_n}, \quad (13)$$

which describe the pressure distributions in the interparticle space.

Here ν_{jn}, j= $\overline{1,\infty}$; $n=\overline{0,\infty}$ – the roots of transcendental equation (10).

$\eta_k=\dfrac{(2k+1)\pi}{2R_1}$, $k=\overline{0,\infty}$ – are the roots of equation $ch\left(\sqrt{\dfrac{s}{b_2}}R_1\right)=0$, ($s=i\eta$, I – imaginary unit),

$\mu_k=\dfrac{(2k+1)\pi}{2R_2}$, $k=\overline{0,\infty}$ – are the roots of equation $ch\left(\sqrt{\dfrac{s}{b_3}}R_2\right)=0$, ($s=i\mu$),

$\lambda_n=\dfrac{2n+1}{2h}\pi$ – are the spectral numbers of integral Fourier transformation (Sin-Fourier).

Substituting into formulas (7) the analytical expression of pressure distributions in the interparticle space $P_1(t,z)$, calculated according to (13), we obtain the final expressions for determining the time-space distributions of pressures $P_2(t,x,z)$ and $P_3(t,x,z)$ in the spaces of nanoporous particles: intraparticle spase 2 and intraparticle spase 3 in accordance.

Numerical modelisation and discussion. As a part of the simulation stage, a special software complex was developed to study the internal kinetics processes of filtration in multidimensional nanoporous particle media. Software complex was developed using a modern approach to software design and software engineering best practices.

Simulation results of the filtration kinetics process study are shown below. The process parameters used in simulations are next: h=0.01m, R_1=0.008 m, R_2=0.004 m, b_1 = 10^{-7} m^2/s, b_2 = 2 10^{-7} m^2/s, b_3 = 10^{-8} m^2/s, β_1 = 0.1, β_2 = 0.15, ε = 0.5. Simulations assumed that the studied media consists of two types of multidimensional nanoporous particles of different kinetic properties.

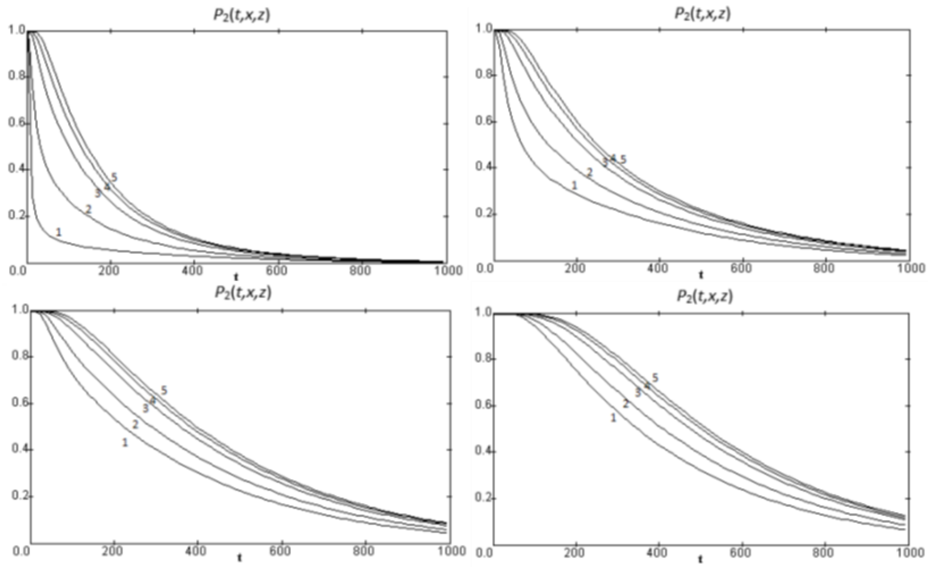

Figure 2. Distribution of dimensionless pressure in the intraparticles space1 $P_2(t,x,z)$ versus time t, [s] in different sections of dimensionless layer: a) Z=0.05; b) Z=0.25; c) Z=0.5; d) Z=1 (Z=z/h); 1 – X=1.0 2 – X=0.8; 3 – X=0.6; 4 – X=0.4; 5 – X=0.05 (X=x_1/R_1)

Figure 2 shows the dimensionless liquid pressure profiles inside the porous particles of first type $P_2(t,x,z)$ in time t[s]. The temporal pressure profiles were simulated for different layer sections: Z=1 (top of layer), Z=0.5 and Z=0.25 (a middle sections of layer), and Z=0 (surface of the filter medium. In the proposed images are clear to observe that liquid pressure is higher in the center of particles (X=0.05) and decline in direction of liquid expulsion on a particles surface $X=1$ ($x_m = R_m$). At the particles edge the pressure in micropores tends to the pressure in macropores $P_1(t,z)$. Also, it is worth to note, that liquid pressure declines rapidly on the particles surface (X=1) than in the middle sections (0.4, 0.6, 0.8) or particles center (X=0.05).

The difference between the temporal pressure profiles becomes more significant for particles located on top of the later (Z=0). However, even in sections close to the central axe of particles (X=0), the liquid pressure drops rather rapidly.

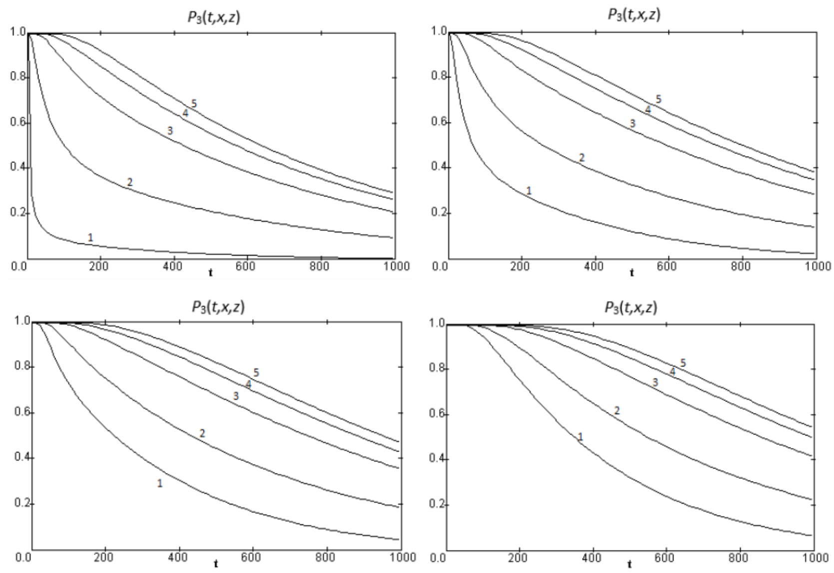

Figure 3. Distribution of dimensionless pressure in the intraparticles space2 $P_3(t,x,z)$ versus time t, [s] in different sections of dimensionless layer: a) Z=0.05; b) Z=0.25; c) Z=0.5; d) Z=1 (Z=z/h); 1 – X=1.0 2 – X=0.8; 3 – X=0.6; 4 – X=0.4; 5 – X=0.05 (X=x_2/R_2)

Figure 3 shows the temporal profiles of dimensionless liquid pressure inside of porous particles of second type (small) in time t[s]. Same as before, the temporal pressure profiles were simulated for four different sections of media layer: Z=1, 0.25, 0.5 and 0.05. The consolidation coefficient for these types of particles characterizes less destroyed cellular tissue compared to the particles of the first type. Like in a previous example, the presented profiles show liquid pressure drops on the surface of particles (X=1) are more rapid than for sections close to the particle's center (X=0.05), and overall decline is more significant when Z leads to 0. However, appreciable retardation of liquid pressure drop can be detected in micropores of particles.

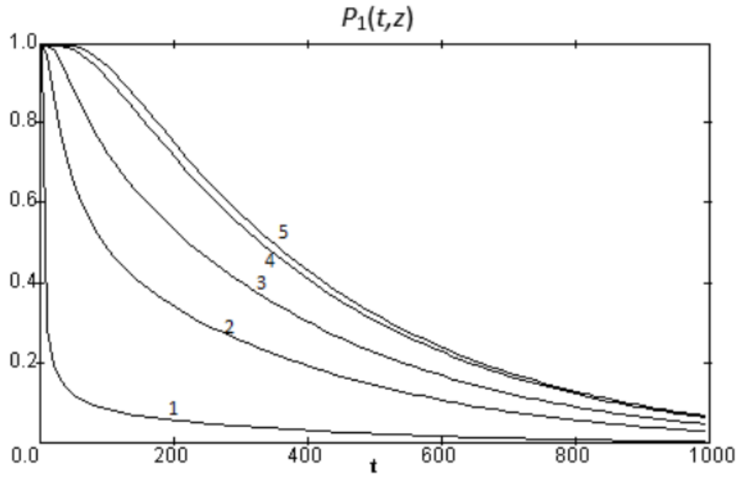

Figure 4. Distribution of dimensionless pressure in the interparticles space $P_1(t,z)$:
1 – Z = 0.05, 2 – Z = 0.3, 3 – Z = 0.5, 4 – Z = 0.7; 5 – Z=1.0 (Z=z/h)

Figure 4 shows distributions of pressure profiles in interparticles space $P_1(t,z)$ at different sections of nanoporous media. Fifth profiles were simulated corresponding to different sections of porous media. Pressures in all layers begin from full saturation and eventually go to almost complete depletion. As we can observe, pressure profiles are not evenly distributed. And most dramatic pressure drop happened for Z=0.05, near the bottom of the filtration media. At the same time, layers located upper keep pressure for a longer period of time, which is an indicator of more saturation.

Conclusions. Phenomenological model of solid-liquid expression from liquid containing nanoporous materials is formulated representing the layer of particles as a bi-porous system with interparticle and intraparticle networks for liquid flowing. The filtration-consolidation equations were formulated for both intrerparticle and two intraparticle networks considering the pressure profiles. It was supposed for nanoporous media that the interaparticles network forms the first porosity with low storage capacity, while the intraparticle network form a two second porosity with high storage capacity.

Analytical and numerical and solutions for pressure distribution and consolidation coefficient were obtained for a real nanoporous material with two different compressibility and permeability characteristics. The results show a slowed down pressure drop in the intraparticle network and a slowing down of nanofiltration kinetics for different-sized nanoporous particles. A special software complex has been built in the framework of science-intensive information technologies for the study of complex processes of nanofiltration in media with various-sized nanoporous particles based on the described mathematical model. The main goals pursued during the design of the software complex were the ability to quickly study nanofiltration processes for scientists, the ability to work on any modern platforms, high-performance numerical modeling and friendly UI/UX. Using software development best practices allowed for a software design that could easily be extended or improved in the future with the ability to add new features and enhancements.

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УДК 519.6

ВИСОКОЕФЕКТИВНІ ІНТЕЛЕКТУАЛЬНІ ІНФОРМАЦІЙНІ ТЕХНОЛОГІЇ ДЛЯ ДОСЛІДЖЕННЯ СИСТЕМ ФІЛЬТРАЦІЇ В СЕРЕДОВИЩАХ РІЗНОРОЗМІРНИХ НАНОПОРИСТИХ ЧАСТИНОК

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Резюме. *Запропоновано інформаційну технологію дослідження нанопористих систем фільтрації, що базується на раніше розробленій феноменологічній моделі двофазного та дворівневого транспорту «нанофільтрація-консолідація» в системі «міжчастковий простір – нанопористі частинки», який враховує складний зворотний зв'язок-взаємодію внутрішнього потоку адсорбованої речовини з нанопор* *сферичних частинок і масового потоку речовини, що знаходиться в міжчастковому просторі. Нанопористе середовище розглядається як багаторівнева пориста система з міжчастинковими та внутрішньочастинковими мережами пор і каналів, що використовуються в якості траспортних потоків для рідини. В свою чергу, частинки середовища містять рідину з різних хімічних компонентів, та утворюють нанопористий шар, що піддається одновимірному стисненню. Частиники розділені пористою мембраною. Шар частинок вважається двопористим середовищем: системи макропор у міжчастинковому просторі та системи нанопор у внутрішньочастинкових просторах, яка включає два підпростори частинок різного розміру.*

На етапі числового моделювання розроблено спеціальний програмний комплекс для дослідження внутрішньої кінетики процесів фільтрації в середовищах з різнорозмірними нанопористими частинками. Програмне забезпечення створено з використанням сучасного підходу до розроблення програмного забезпечення та з урахуванням найкращих практик програмної інженерії.

Результати проведеного чисельного моделювання показують сповільнене падіння тиску у внутрішньочастинковій мережі та уповільнення кінетики консолідації для сеоедовищ з різнорозмірними нанопористими частинками. В рамках наукоємних інформаційних технологій для дослідження процесів фільтрації в середовищах з різнорозмірними нанопористими частинками на основі описаної математичної моделі побудовано спеціальний програмний комплекс. Основними цілями розроблення такого комплексу були можливість швидкого вивчення процесів фільтрації для науковців, можливість роботи на будь-яких сучасних платформах, високопродуктивне чисельне моделювання та зручний користувацький інтерфейс. Використання сучасних практик розроблення програмного забезпечення дозволило розробити архітектуру програмного забезпечення, яку можна легко розширити або вдосконалити в майбутньому з можливістю додавання покращень або нового функціоналу.

Ключові слова: *процеси фільтрації, чисельне моделювання, паралельні обчислення, наукомісткі технології, середовища з різнорозмірними нанопористими частинками*.

https://doi.org/10.33108/visnyk_tntu2022.04.016 *Отримано 20.12.2022*