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M.R. PETRYK, D.M. MYKHALYK, V.M. BREVUS, I.V. GOYANYUK
Ternopil National Ivan Pul'uj Technical University

HIGH-PERFORMANCE INFORMATION TECHNOLOGIES TO STUDY FILTRATION PROCESSES IN MEDIA WITH VARIABLE-SIZED NANOPOROUS PARTICLES

This study presents mathematical solutions for the pressure distribution and consolidation coefficient within a nanoporous material characterized by varying compressibility and permeability properties. The mathematical model of nanoporous filtration systems is founded on a phenomenological model developed by the authors. This model encapsulates the intricate dynamics of a two-phase and two-level transport process, known as nanofiltration-consolidation. To solve the defined mathematical problem analytically, the operational Heaviside's method where employed in composition with Laplace integral and Fourier integral transformations. The application of the finite integral cos Fourier transform allowed to get analytical representations for pressure profiles both in interparticle and intraparticle spaces as a function of particle position within media, particles radius, and total time.

To advance understanding of complex nanofiltration processes occurring within media containing nanoporous particles of varied sizes, a specialized software complex has been engineered. The adherence to software development best practices has rendered the software design highly adaptable, allowing for effortless future extensions and improvements. This, in turn, empowers the software with the capacity to seamlessly incorporate new features and enhancements.

As a part the simulation phase, a constructed software suite was used to explore the internal kinetics of filtration processes within multidimensional nanoporous particle media. Numerical modelization results reveal insight into internal processes, such as pressure drop within the intraparticle network, leading to a notable deceleration in nanofiltration kinetics, specifically in relation to nanoporous particles of differing sizes. Among them, the consolidation coefficients indicate that particles of the second-type have a less destroyed cellular structure compared to particles of the first-type. The simulated profiles illustrate that liquid pressure experiences rapid drops at the surface of the particles in contrast to the sections closer to the center of the particles. Furthermore, a more substantial overall decline occurs as vary-sized particles approach the media edge. In the other hand, a noticeable slowing down of the liquid pressure drop can be observed in the micropores of the particles.

Key words: filtration processes, numerical modeling, parallel computing, nanoporous particles media.

М.Р. ПЕТРИК, Д.М. МИХАЛИК, В.М. БРЕВУС, І.В. ГОЯНЮК
Тернопільський національний технічний університет імені Івана Пулюя

ВИСОКОПРОДУКТИВНІ ІНФОРМАЦІЙНІ ТЕХНОЛОГІЇ ДЛЯ ДОСЛІДЖЕННЯ ПРОЦЕСІВ ФІЛЬТРАЦІЇ В СЕРЕДОВИЩАХ ІЗ НАНОПОРИСТИМИ ЧАСТИНКАМИ РІЗНОГО РОЗМІРУ

В дослідженні представлено розв'язки математичної моделі для розподілів тиску та коефіцієнту консолідації всередині нанопористого матеріалу, що характеризується різними властивостями стисливості та проникності. Математична модель фільтрації в нанопористому середовищі базується на феноменологічній моделі, розробленій авторами. Ця модель охоплює складну динаміку двофазного та дворівневого процесу транспортування, відомого як нанофільтрація-консолідація. Для відшукання розв'язку поставленої математичної задачі аналітично використовувався операційний метод Хевісайда в поєднанні з інтегральними перетвореннями Лапласа та перетвореннями Фур'є. Застосування скінченного інтегрального перетворення Фур'є cos дозволило отримати аналітичні представлення для профілів тиску як у міжчастинковому, так і внутрішньочастинковому просторах у вигляді функції від положення частинки в середовищі, радіуса частинки та загального часу.

Для покращення розуміння складних процесів нанофільтрації, що відбуваються в середовищах нанопористих частинки різного розміру, був розроблений спеціалізований програмний комплекс. Дотримання найкращих практик розробки програмного забезпечення зробило дизайн програмного забезпечення дуже адаптивним, дозволяючи легко розширювати та вдосконалювати його за потреби. Це, у свою чергу, надало програмному забезпеченню можливість безперешкодно включати нові функції та вдосконалення.

Як частина етапу моделювання, розроблений пакет програмного забезпечення використовувався для дослідження внутрішньої кінетики процесів фільтрації в багатовимірних нанопористих середовищах. Результати чисельного моделювання відкривають розуміння внутрішніх процесів, таких як падіння тиску всередині мережі частинок, що призводить до помітного уповільнення кінетики нанофільтрації, особливо щодо нанопористих частинок різного розміру. Зокрема, коефіцієнти консолідації вказують що частинки другого типу мають менш зруй-

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нувану клітинну структуру у порівнянні з частинками першого типу. Змодельовані профілі показують, що тиск рідини швидко падає на поверхні частинок на відміну від ділянок, розташованих ближче до центру частинок. Крім того, більш істотне загальне зниження відбувається, коли частинки різного розміру наближаються до краю середовища. З іншого боку, в мікропорах частинок можна спостерігати помітне уповільнення падіння тиску рідини.

Ключові слова: процеси фільтрації, чисельне моделювання, паралельні обчислення, середовища з нанопористими частинками.

Introduction

In various domains such as environmental protection, emission reduction, medicine, and the filtration of liquids or gases, the design of intricate systems and processes necessitates the creation of high-performance information systems. These systems are crucial for conducting research based on scientifically grounded mathematical models that provide a robust physical basis for understanding the composition of system elements, their interconnections, and the parameters that dictate their effectiveness and functionality.

The proposed information technology for the investigation of nanoporous filtration systems is founded on a phenomenological model previously developed by the authors. This model encapsulates the intricate dynamics of a two-phase and two-level transport process, known as “nanofiltration-consolidation”, occurring within the system’s “interparticle space – nanoporous particles”. It comprehensively addresses the complex interplay between the internal flow of adsorbed substances from the nanopores of spherical particles and the mass flow of substances residing in the interparticle space [1, 2].

Problem Formulation

The nanoporous medium is characterized as a multi-level porous system featuring networks for swift fluid flows within both interparticle and intraparticle spaces. Within this context, we examine nanoporous particles containing a liquid substance comprised of various chemical constituents.

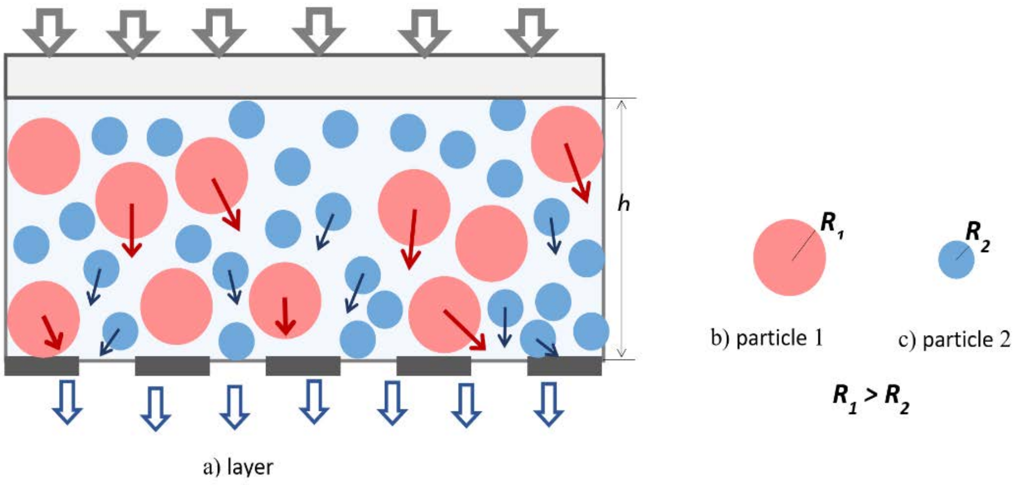

Fig. 1. Liqued flow interactions in a two-level nanopores system:
(1) – intraparticle space and (2) – intraparticle space spaces

These particles collectively constitute a nanoporous layer, which undergoes one-dimensional compression (see Fig. 1). Substance flows intermingle across all the spaces under consideration. The separation of nanoporous particles is facilitated by a porous membrane. Each layer of particles is regarded as a two-pore medium.

In Figure 1, two levels of the elementary volume are depicted: Level 1(a) corresponds to the system of macropores in the interparticle space, while Level 2 (b and c) pertains to the system

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of nanopores within intraparticle spaces. This second level encompasses two subspaces containing particles of different sizes: intraparticle space 1, which consists of nanoporous particles with a radius of at least R_1, and intraparticle space 2, encompassing nanoporous particles with a radius of at least R_2 (where $R_1 > R_2$).

Mathematical Model Definition

The intricate system of nanofiltration and nano diffusion within spaces containing nanoporous particles of varying sizes is described by a mathematical model. This model considers specific physical factors and feedback interactions, and it is expressed as a system of boundary value problems comprising partial differential equations. These equations pertain to the three interconnected spaces defined in relation to the liquid phase, encompassing the interparticle space and two intraparticle spaces.

Consolidation** equation **in interparticle space. To find the solution to the equation for layers with variable-sized nanoporous particles in the domain $D_1 = \{(t,z) : t > 0, \quad 0 < z < h\}$

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

with initial condition

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

and boundary conditions

$$P_1(t,z)|_{z=0} = 0, \quad \frac{\partial P_1}{\partial z}\Big|_{z=h} = 0 \tag{3}$$

Consolidation equations for particle. To find the solutions of the equations for the nanoporous particles (radius R_i) in the domain

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

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

with initial condition

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

and boundary conditions

$$\frac{\partial P_i}{\partial x_j}\Big|_{x_j=0} = 0, \quad P_i(t, x_j, z)|_{x_j = R_j} = P_1(t,z) \tag{6}$$

Here: 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 of various size) in accordance, b_1 – consolidation coefficient in interparticle space, b_2, b_3 – consolidation coefficients in intraparticle space for various particles, β_1, β_2 – elasticity factor of various particles, h – layer thickness, R_1, R_2 – radius of various particles.

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Finding Analytical Solution

To solve the defined mathematical problem analytically, we employ the operational Heaviside's method, Laplace integral, and Fourier integral transformations. The application of the finite integral Fourier transform (cos) is discussed in [3, 4].

$$F_c\left[P_i\left(t,x_j,z\right)\right]=\int_0^{R_j}P_i(t,x_j,z)\vartheta\left(x_j,\eta_{m_j}\right)dx_j=\int_0^{R_j}P_i(t,x_j,z)\cos\eta_{m_j}x_jdx_j\equiv P_{im_j}(t,z),$$

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

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

where: $\vartheta\left(x_j,\eta_{m_j}\right)=\cos\eta_{m_j}x_j$, $\eta_{m_j}=\dfrac{2m_j+1}{2R_j}\pi$, $m_j=\overline{0,\infty}$ spectral functions and spectral numbers of the integral Fourier cos-transformation.

Consiquentionaly, solutions of the problems B_1, B_2 are obtained:

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

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

By substituting the expressions from equation (7) into the consolidation equation (1), and through a sequence of transformations, and subsequently applying the integral Laplace transform as outlined in [3], and the finite integral Fourier transform (sin), the problem (1)–(3) is addressed.

$$F_s\left[P_1^*(s,z)\right]=\int_0^hP_1^*(s,z)\cdot V(z,\lambda_n)\,dz=\int_0^hP_1^*(s,z)\cdot\sin\lambda_nzdz=P_{1,n}^*(s)$$

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

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

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

Applying the integral operator of the inverse integral Laplace transformation to expression (8) we obtain in [5] and taking into account series [3] we finally obtain solution for pressure P_1

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

After introducing the notation

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

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

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

here L^{-1} is integral operator of inverse Laplce transformation and * is an operator of both functions convolution. As follows, by making replacements $i\sqrt{s} = \nu$ and $s = -\nu^2$, we obtain next equation:

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

And based on Heviside's theorem one get the equation of back to original [4]:

$$\cdot L^{-1}\left[\frac{1}{s + b_1\lambda^n + \beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)}\right] = \\ = \sum_{\square=0}^{\infty}\left.\frac{e^{st}}{\frac{d}{ds}\left[s + b_1\lambda^n + \beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)\right]}\right|_{s=-\nu^2_{\square n}} \tag{11}$$

where ν_{jn}, j=$\overline{1,\infty}$; $n = \overline{0,\infty}$ are roots of the transcendental equation above.

After transforming the denominator, expression (11) will have the final form:

$$\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2 t}}{1+\Phi\left(\nu_{jn}\right)}$$

Finally, the analytical solution fort P_1 has a form of equation:

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$$P_1(t,z) = P_E \frac{2}{h}\sum_{n=0}^{\infty}\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2 t}}{\Phi(\nu_{jn})}\left[1-\beta_1\varepsilon\frac{2}{R_1^2}\sum_{k=0}^{\infty}\frac{1-e^{-b_2\left(\eta_k^2-\frac{\nu_{jn}^2}{b_2}\right)t}}{\left(\eta_k^2-\frac{\nu_{jn}^2}{b_2}\right)} - \beta_2(1-\varepsilon)\frac{2}{R_2^2}\sum_{k=0}^{\infty}\frac{1-e^{-b_3\left(\mu_k^2-\frac{\nu_{jn}^2}{b_3}\right)t}}{\left(\mu_k^2-\frac{\nu_{jn}^2}{b_3}\right)}\right]\frac{\sin\lambda_n z}{\lambda_n} \tag{12}$$

The equation represent liquid pressure distribution in the interparticle space.

ν_{jn}, $j=\overline{1,\infty}$; $n=\overline{0,\infty}$ are the roots of the 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).

Numerical modelization and discussion

During the simulation phase, a dedicated software suite was created to explore the internal kinetics of filtration processes within multidimensional nanoporous particle media. This software complex was developed in adherence to modern software design principles and best practices in software engineering [6, 7].

The simulation results of the filtration kinetics process are presented below. The simulations employed the following parameters: $h = 0.01$ m, $R_1 = 0.008$ m, $R_2 = 0.004$ m, $b_1 = 10^{-7}$ m²/s, $b_2 = 2\ 10^{-7}$ m²/s, $b_3 = 10^{-8}$ m²/s, $\beta_1 = 0.1$, $\beta_2 = 0.15$, and $\varepsilon = 0.5$. It was assumed in the simulations that the media under investigation comprised two types of multidimensional nanoporous particles with distinct kinetic properties.

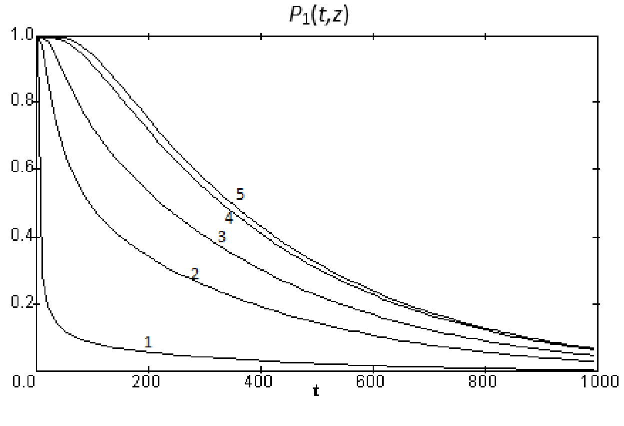

Fig. 2. Distribution of dimensionless pressure in interparticle space $P_1(t,z)$:
1 – Z = 0.05, 2 – Z = 0.3, 3 – Z = 0.5, 4 – Z = 0.7; 5 – Z = 1.0 (Z=z/h)

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Figure 2 presents pressure profile distributions within the interparticle space, denoted as $P_1(t, z)$, across various sections of nanoporous media. Five profiles were simulated, each corresponding to different sections of the porous media. It's essential to note that pressures in all these layers initiate from a state of full saturation and gradually progress toward near-complete depletion.

It's evident from the figures that the pressure profiles are not uniformly distributed. The most significant pressure drop occurs at Z = 0.05, near the lower part of the filtration media. In contrast, layers situated higher up maintain pressure for a more extended duration, signifying a higher level of saturation in those regions.

Figure 3 illustrates dimensionless liquid pressure profiles within porous particles of the first type, denoted as $P_2(t, x, z)$, as a function of time (t [s]). The temporal pressure profiles were simulated for various layer sections, including Z = 1 (at the top of the layer), Z = 0.5, and Z = 0.25 (representing middle sections of the layer), and Z = 0 (at the surface of the filter medium).

From the provided images, it is evident that the liquid pressure is highest at the center of the particles (X = 0.05) and decreases as it moves towards the liquid expulsion point on the particle surface at X = 1. Notably, at the edge of the particles, the pressure in the micropores approaches the pressure in the macropores, denoted as $P_1(t, z)$. Additionally, it's noteworthy that the liquid pressure experiences a more rapid decline on the particle's surface (X = 1) compared to the middle sections (X = 0.4, 0.6, 0.8) or the central axis of the particles (X = 0.05).

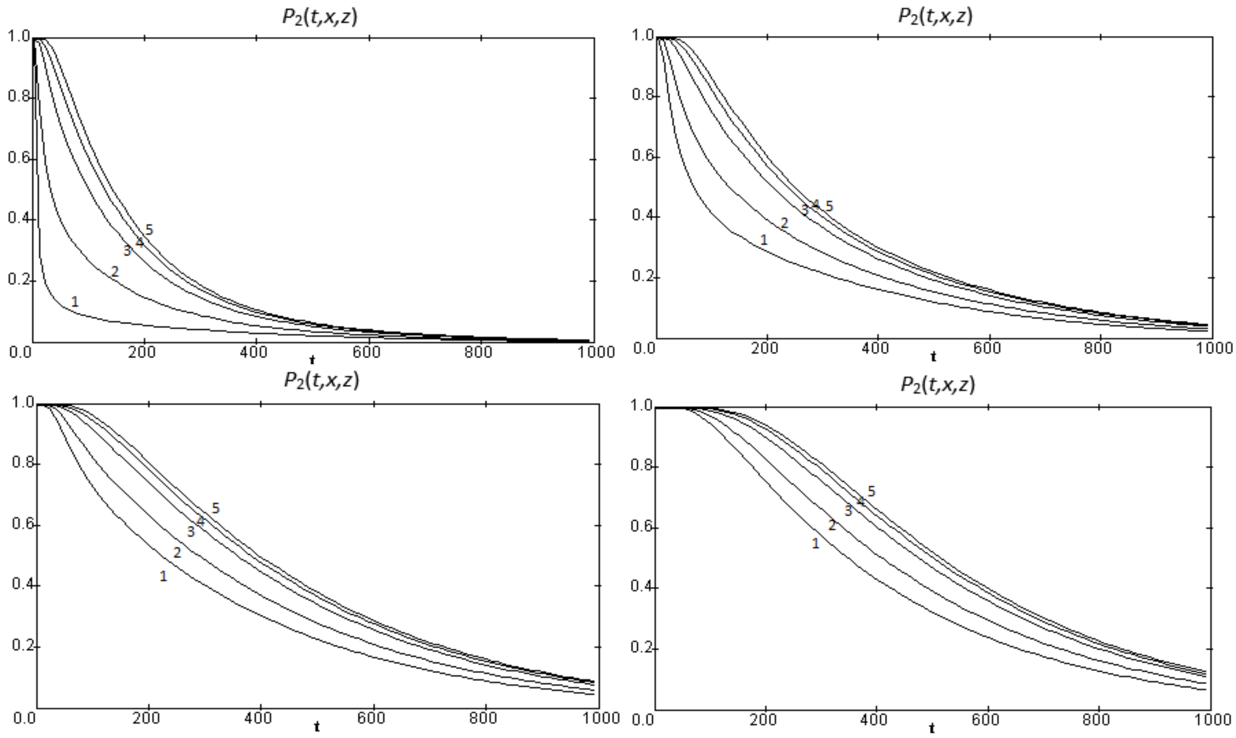

Fig. 3. Distribution of dimensionless pressure in intraparticles space $P_2(t,x,z)$ in time (t [s]) for sections: a) Z = 0.05; b) Z = 0.25; c) Z = 0.5; d) Z = 1 (Z = z/h); 1 – X = 1.0; 2 – X = 0.8; 3 – X = 0.6; 4 – X = 0.4; 5 – X= 0.05 (X = x_1/R_1)

The discrepancy in temporal pressure profiles becomes more pronounced for particles situated at the top of the layer (Z = 0). However, even in sections near the central axis of the particles (X = 0), the liquid pressure decreases rather swiftly.

In Figure 4, we depict the temporal profiles of dimensionless liquid pressure within porous particles of the second type (small). Similar to the previous example, these temporal pressure profiles were simulated for four distinct sections of the media layer: Z = 1, 0.25, 0.5, and 0.05.

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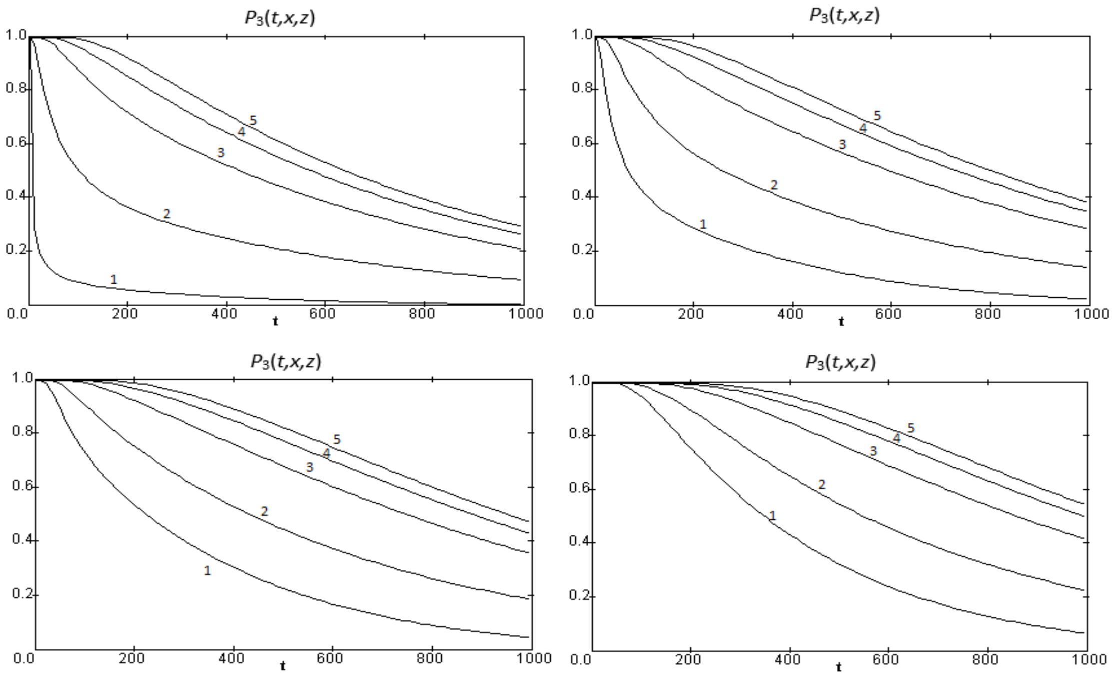

Fig. 4. Distribution of dimensionless pressure in the intraparticles space $P_3(t,x,z)$ in time (t [s]) for sections: a) Z = 0.05; b) Z = 0.25; c) Z = 0.5; d) Z = 1 (Z = z/h); 1 – X = 1.0; 2 – X = 0.8; 3 – X = 0.6; 4 – X = 0.4; 5 – X = 0.05 (X = x_2/R_2)

The consolidation coefficient for these second-type particles signifies a less disrupted cellular structure compared to the first-type particles. As observed in the previous instance, the presented profiles illustrate that liquid pressure experiences rapid drops at the surface of the particles (X = 1) in contrast to the sections closer to the center of the particles (X = 0.05). Furthermore, a more substantial overall decline occurs as Z approaches 0. Nonetheless, it’s worth noting that a noticeable slowing down of the liquid pressure drop can be observed in the micropores of the particles.

Conclusions

The mathematical solution has been constructed for the liquid pressure distribution and consolidation coefficient in a real nanoporous material characterized by distinct compressibility and permeability properties. These results indicate a deceleration in pressure drop within the intraparticle network and a corresponding slowdown in nanofiltration kinetics for nanoporous particles of different sizes.

To facilitate the study of complex nanofiltration processes within media featuring various-sized nanoporous particles, a specialized software complex was developed using cutting-edge science-intensive information technologies, closely aligned with the described mathematical model. Key objectives in designing this software complex included enabling rapid research into nanofiltration processes for scientists, compatibility with modern platforms, high-performance numerical modeling, and a user-friendly interface

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Петрик Михайло Романович – д.ф.-м.н., завідувач кафедри програмної інженерії Тернопільського національного технічного університету імені Івана Пулюя. E-mail: Mykhaylo_Petryk@tu.edu.te.ua, ORCID: 0000-0001-6612-7213.

Михалик Дмитро Михайлович – к.т.н., доцент кафедри програмної інженерії Тернопільського національного технічного університету імені Івана Пулюя. E-mail: D.Mykhalyk@gmail.com, ORCID: 0000-0001-9032-695X.

Бревус Віталій Миколайович – к.т.н., доцент кафедри програмної інженерії Тернопільського національного технічного університету імені Івана Пулюя. E-mail: v_brevus@tntu.edu.ua, ORCID: 0000-0002-7055-9905.

Гоянюк Іван Васильович – здобувач кафедри програмної інженерії Тернопільського національного технічного університету імені Івана Пулюя. E-mail: ivan.goyanyuk@gmail.com, ORCID: 0000-0003-3760-1929.

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Petryk Mykhaylo Romanovych – Doctor of Physical and Mathematical Sciences, Head of Software Engineering Department of Ternopil National Ivan Pul'uj Technical University. E-mail: Mykhaylo_Petryk@tu.edu.te.ua, ORCID: 0000-0001-6612-7213.

Mykhalyk Dmytro Mykhailovych – Ph.D in Technical Sciences, Senior Lecturer at the Software Engineering Department of Ternopil National Ivan Pul'uj Technical University. E-mail: D.Mykhalyk@gmail.com, ORCID: 0000-0001-9032-695X.

Brevus Vitaly Mykolaiovych – Ph.D in Technical Sciences, Senior Lecturer at the Software Engineering Department of Ternopil National Ivan Pul'uj Technical University. E-mail: v_brevus@tntu.edu.ua, ORCID: 0000-0002-7055-9905.

Goyanyuk Ivan Vasylovych – Postgraduate Student of Software Engineering Department of Ternopil National Ivan Pul'uj Technical University. E-mail: ivan.goyanyuk@gmail.com, ORCID: 0000-0003-3760-1929.

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