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NUMERICAL MODELING OF LIQUID SOLUTION FILTRATION IN A CYLINDRICAL POROUS FILTER

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A mathematical and numerical model is presented for the process of liquid solution filtration in a cylindrical porous filter. The model is based on the Brinkman–Darcy equations, describing fluid motion in a porous medium with porosity and permeability linked through the Kozeny–Carman relation. The transport of dissolved substances is governed by the advection–diffusion–reaction system, complemented by the LDF kinetics and the Langmuir isotherm for adsorption. The model also incorporates a clogging (colmatation) equation that accounts for particle deposition and temporal reduction of filter porosity. A finite-difference numerical algorithm with iterative pressure correction using the conjugate gradient method is developed, ensuring stability according to the Courant–Friedrichs–Lewy criterion. The proposed approach enables analysis of the coupled hydrodynamic, mass transfer, and adsorption phenomena, allowing for assessment of filtration efficiency and prediction of filter lifespan in liquid purification systems.

Keywords: hydrodynamics of porous media, mass transport, Brinkman–Darcy equations, numerical approximation, liquid purification.

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1 Introduction

One of the priority areas of modern environmental and engineering problems is the conservation of water resources, the effective removal of industrial and domestic pollutants, and ensuring the quality of drinking water. Porous filters (granular filtration systems, biofilters, membrane systems equipped with filter layers, etc.) are widely used in many industrial and utility applications of these problems. However, for a complete understanding of the actual behavior of filters, a physico-mathematical model is required that takes into account the processes of flow hydraulics, substance transport, adsorption kinetics, and blockage (clogging).

In this work, the processes occurring in a porous filter with a cylindrical geometry (axial symmetry) - fluid flow and pressure distribution, convective-diffuse transport of several components, adsorption and its kinetics, as well as clogging and interaction with the membrane caused by large particles - are mathematically modeled as a single system. When constructing the model, the Brinkman-Darcy formulas (a tool describing the transition from the traditional Darcy approach to the Stokes state) allow for a better description of hydraulic behavior; the relationship between permeability and porosity is introduced using the Kozeny-Carman formula; convection-diffusion-reaction (ADR) equations are used for substances in the liquid phase; LDF kinetics and Langmuir isotherm are used to describe adsorption processes; colmatation is included in the model through

particle deposition and decrease in porosity over time; and membrane surface massing and permeation are expressed through special boundary conditions.

This work not only provides a mathematically perfect model, but can also be applied in practice when optimizing the design of water treatment plants, assessing their service life, and developing operational strategies. The interaction of surface and groundwater is of great interest in land reclamation, engineering hydrology, and hydrogeology. This study is aimed at modeling unsteady fluid filtration in a sandwich-type reservoir system, which is a particularly relevant topic for Uzbekistan, where such soil structures are widespread. A mathematical model of filtration is formed using partial differential equations of parabolic type, subject to boundary conditions. An analytical solution was obtained by applying the Laplace transform. Computational experiments were conducted to analyze the pressure change along the length of the filtration layers in inelastic mode. The results showed that the pressure in both layers increases exponentially, and water exchange along the boundary strongly depends on the piezoconductivity of the strongly permeable layer and the filtration coefficient of the weakly permeable layer.

The research provides an analytical solution to the problem of filtration in a sandwich-type reservoir system, including the determination of pressure distribution in a low-permeability layer. In addition, a new generalized formula for managing well galleries has been obtained. The developed mathematical framework allows for the development of layout and capacity schemes for vertical drainage wells, thereby offering practical tools for preventing flooding of irrigated and non-irrigated areas, protecting groundwater from pollution sources, and isolating already contaminated zones [1].

A mathematical model and an effective numerical algorithm have been developed for a comprehensive investigation of the technological process of filtration of liquids and ionized solutions. The model takes into account the change in filtration rate, the change in the concentration of the suspension inside the column and at the outlet, the formation of a sediment layer on the filter surface, the deposition of gel particles in the filter holes, the increase in pressure in the column and sediment layer, as well as other physical and mechanical properties of the filtered liquid. Computational experiments were conducted, the results of which were presented graphically to support analysis and decision-making on the operating modes of the filtration unit, depending on the characteristics of the suspension and other influencing factors.

Numerical simulations have shown that the baro diffusion coefficient is one of the main parameters in ion-exchange filtration of ionized solutions. An increase in this coefficient accelerates the rate of ion exchange in the solution and filter medium, which reduces the service life of the filter column and prevents the full utilization of the filter's ion exchange capacity. The results showed that the formation of a cake layer on the filter surface significantly affects the flow rate, the output concentration, and the increase in hydraulic pressure inside the column. In addition, it was established that the initial flow rate of the liquid into the filter column and the thickness of the filter medium play an important role. It has been shown that a decrease in the initial flow rate significantly alters the main indicators of the process, in particular, the concentration of the solution on the filter surface, the output concentration of the filtrate, and the rate of precipitation of gel particles in the filter holes [2].

Filtration plays a crucial role in the stability and operation of hydraulic structures. This can lead to serious consequences, including water losses from reservoirs, the effect of back pressure caused by filtration, and volumetric hydrodynamic forces inside the structure. In engineering practice, isotropic filtration is often investigated, where the

material exhibits uniform conductivity in all directions. Under the hydraulic head created by the dam, water flows along the dam body from the top to the flow side. The upper limit of this filtration process is determined by the depression curve. When a depression curve appears on the lower slope, filtration continues under residual pressure, forming a drain along the slope surface. This leak carries soil particles from the dam body; this process is called suffusion. Supfusion increases permeability, which can lead to a drop in the downstream flow, which poses a direct threat to the integrity of the dam, and ultimately to failure. The article examines the problems of mathematical modeling of plane-parallel isotropic fluid filtration [3].

The study, along with formulas for determining fluid flow in a well, examines the laws of pressure distribution regulation under direct radial flow conditions, taking into account horizontal and vertical directions [4].

This study examines the interaction of process properties such as fluid concentration and sludge contamination with environmental parameters such as porosity, filtration, diffusion, and mass permeability. The analysis is carried out using the example of liquid purification in magnetic and sorption filters. An algorithm for the numerical-asymptotic approximation of the control model problem has been developed, which is characterized by a system of nonlinear, singularly perturbed differential equations of the "convection-diffusion-mass transfer"type. It has been shown that the obtained relationships (formulas) are effective for optimizing water treatment processes and increasing the overall productivity of treatment systems, since they allow determining the protection time, filter sizes, and other key parameters in cases where convection and sorption prevail over diffusion and desorption - a situation characteristic of most filtration systems. On this basis, a computer experiment was conducted, demonstrating the advantages of the proposed model over classical approaches [5].

The article explores the application of mapping methods adapted to boundary value problems for calculating filtration processes in horizontal system drainage systems, especially when drains are installed at different depths. When analyzing filtration regimes in soils containing free boundaries (depression curves) and drainage-type intervals, special attention is paid to approaches combining imaginary domains with quasi-conformal maps for solving nonlinear boundary conditions. As a visual example, the authors constructed a hydrodynamic flow network, calculated the flow velocity to the drainage, determined the cross-section, and obtained other key process characteristics. An algorithm for the numerical solution of nonlinear boundary value problems using quasi-conformal mapping in domains bounded by two equipotential and two stream boundaries has been developed, one of which is represented by an unknown (free) curve with fixed and free endpoints. Numerical experiments confirmed the effectiveness of the proposed models and algorithms for simulating nonlinear filtration processes occurring in horizontal drainage systems requiring a relatively small number of repetitions ($k = 141$) [6].

This research is aimed at developing a mathematical model for nonlinear filtration of fluids formed in a layered medium. The analysis studies the flow velocity between layers as a function of the properties of the layer and the properties of the liquid. In addition, digital algorithms were developed to support computational experiments and confirm the proposed model [7].

This article presents a detailed mathematical model for the development of low-permeability reservoirs using paired horizontal channels in the presence of cracks caused by hydraulic fracturing. Hydraulic fracturing remains one of the most effective ways to increase well productivity, especially in geologically complex formations. However, its

effectiveness is often limited by insufficient understanding of the mechanisms of fluid flow within the filtration channels formed as a result of high-pressure fluid injection. To solve this problem, in the study, a simplified model is considered, modeled as the only hypothetical well in which a system of horizontal wells simultaneously performs water injection and oil production. The problem of the movement of the oil-water interface between hydraulic fractures in a reservoir with low permeability is analyzed.

The proposed model describes two-phase (oil-water) filtration based on mass balance equations and Darcy's law for each phase, thereby allowing for the study of injection and production processes in the wellbore and the surrounding reservoir section. The modeling results emphasize the influence of the fracture diameter on the pressure distribution and water saturation. These findings allow for the determination of optimal operating modes for injection wells and the prediction of water rupture and associated well production rates using numerical methods characterized by low computational error. [8]

In the study of fluid dynamics and porous media, nonlinear filtration of fluid in two-layer systems presents a significant challenge, requiring a solid mathematical basis for precise description and analysis. This article presents a multi-parameter mathematical model aimed at determining the complexity of filtration processes in a heterogeneous medium, with special attention paid to a two-layer medium. The research is aimed at developing and numerically solving nonlinear filtration problems for structured and unstructured fluids in hydrodynamically coupled multilayer layers with various properties. The proposed models and computational algorithms were validated using a hypothetical dataset and demonstrated their applicability and effectiveness. [9]

This study examines the practical problems associated with fluid flow into wells and groundwater movement in confined layers in basin conditions, paying particular attention to their role in environmental pollution. The main goal is to study the application of complex potentials in assessing well performance in limited areas and to characterize the behavior of production and injection wells in such systems. The study is based on the hypothesis that under natural migration processes and imposed constraints, streamlines and equipotential lines can effectively serve as impermeable boundaries or free surface boundaries. Conformal mapping methods were used to construct complex flow potentials for wells of reservoir configuration. In addition, the work provides a method for determining the maximum permissible well flow, which prevents pollution. The study also establishes the conditions governing the migration of pollutants from a specific source, formed using complex potentials characterizing the flow area [10].

Within the framework of the theory of interacting durations, control equations were obtained to describe the motion of two immiscible fluids in a poroelastic skeleton. The study further explores the stability of the system's solution in a stable state [11].

This article presents a mathematical model of fluid filtration in subsurface formations, developed and numerically solved in the context of electricity generation. The study considers anomalously structured and Newtonian fluids as filtration objects. Computational algorithms are built using iterative procedures, as well as direct and stream differential cleaning methods. A numerical analysis of the problem was carried out, which allows determining the inter-reservoir flow velocity and the positions of the fault boundaries, taking into account the dynamics of reservoir development [12].

The removal of acrylonitrile (AN) from exhaust gas streams by biological treatment methods has recently attracted increasing attention due to their high efficiency. This research is aimed at modeling the removal of AN using a biofilter. Testing of the model was carried out using experimental data obtained from a biofilter column with a yard waste

compost, crushed solid plastics, and thickened urban active clay. The kinetics of biological decomposition of acrylonitrile were first analyzed, and then control equations for the biofilm and air phase were derived under conditions of stable state and constant temperature. Unknown model parameters were evaluated using the least squares optimization method in conjunction with MATLAB-based solutions of system equations.

For the input concentration below 1 g/m^3, the model showed good agreement with experimental observations. Sensitivity analysis showed that the Peclet number, film thickness, and biomass concentration are the most influential factors affecting the biofilter's performance. Therefore, the proposed model provides a valuable tool for designing and optimizing the biofilter. [13]

Anomalous filtration of the same liquid in a porous medium is modeled by differential equations with fractional derivatives, constructed in the Caputo sense. The study examines and numerically solves the filtration problem in a limited homogeneous reservoir, focusing on assessing how abnormal behavior affects filtration properties. The results show that a decrease in the fractional exponent of the derivative in terms of relaxation relative to pressure reduces the pressure distribution to a certain distance from the reservoir boundary, and then increases. Conversely, reducing the order of the derivative in the term gevşeme relative to the filtering rate causes an inverse effect. The dynamics of filtration rate changes accordingly with decreasing fractional orders.

A special case is noted where the relaxation time of the filtration rate exceeds the pressure, including the case when the latter is equal to zero. Under these conditions, the solution of the filtration equation exhibits wave-like behavior. In addition, as the difference between filtration rate and pressure relaxation times increases, the propagation rate of pressure waves decreases. [14]

This study forms and numerically solves the problem of anomalous filtration and transport of dissolved substances in a two-zone medium with a linear source. In the first zone, transport is regulated by anomalous convective-diffusion processes, while in the second zone, it is regulated only by diffusion. The impact of abnormal behaviour on transport characteristics is also assessed. [15]

2 Problem formulation

Below are the equations for a cylindrical porous filter.

Equations for hydraulics (Brinkman-Darcy) (1) - (4):

$$\frac{1}{r}\frac{\partial\left(ru_r\right)}{\partial r}+\frac{\partial u_z}{\partial z}=0. \tag{1}$$

Where: r – radial coordinate[m], distance from the center to the wall, z – vertical coordinate [m], direction from top to bottom, $u_r=u_r\left(r,z,t\right)$ – radial velocity component [m/s], $u_z=u_z\left(r,z,t\right)$ – vertikal velocity component [m/s], θ – angular coordinate [rad], not taken when the axis is symmetrical, $u_\theta\left(r,z,t\right)$ – angular velocity component [m/s], zero due to symmetry.

This equation expresses the equation of conservation of mass - the incompressibility of water. This ensures constant equilibrium between the incoming and outgoing flow volumes and guarantees mass conservation regardless of the pressure inside the filter.

$$-\frac{\mu}{\varkappa\left(\varepsilon\right)}u_r+\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_r}{\partial r}\right)+\frac{\partial^2 u_r}{\partial z}-\frac{u_r}{r^2}\right)-\frac{\partial p}{\partial r}0. \tag{2}$$

Where: μ – dynamic viscosity [Pa·s], for water 0.001 (20 °C da), $\varkappa\left(\varepsilon\right)$ – permeability [m^2], flow capacity, $p=p\left(r,z,t\right)$ – pressure [Pa].

This equation is the radial momentum equation, which governs the radial velocity with the pressure gradient and pore resistance. If the pressure differs from the center to the wall, the fluid flows radially, but pore resistance slows down this movement.

$$-\frac{\mu}{\varkappa(\varepsilon)}u_z + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_z}{\partial r}\right) + \frac{\partial^2 u_z}{\partial z^2}\right) - \frac{\partial p}{\partial z}0. \tag{3}$$

This equation drives the flow with the pressure difference for the axial momentum equation - the main direction of the flow (from top to bottom). Porous resistance and viscosity slow down the flow. Therefore, the flow rate at the outlet changes depending on the pressure difference.

$$\varkappa(\varepsilon) = \frac{\varepsilon^3 d_f^2}{180(1-\varepsilon)^2}. \tag{4}$$

Where: $\varepsilon(r,z,t)$ – porosity, $(0<\varepsilon<1)$, proportion of free space, d_f - filter particle diameter [m].

This equation expresses the Kozeny-Carman formula and relates the internal structure (porosity) of the filter to the flow capacity. In a coarse-grained or more porous filter, the flow passes more easily.

For substance transport (for each $i=1,\ldots,N$), the following equations (5) – (8) are expressed.

$$\begin{aligned}\frac{\partial(\varepsilon c_i)}{\partial t} + \frac{1}{r_r}\frac{\partial}{\partial r} + (rc_i u_r) + \frac{\partial}{\partial z}(c_i u_z) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon D_{i,eff}\frac{\partial c_i}{\partial r}\right) + \\ + \frac{\partial}{\partial z}\left(\varepsilon D_{i,eff}\frac{\partial c_i}{\partial r}\right) - r_{i,\text{bulk}} - a_s r_{i,\text{surf}}.\end{aligned} \tag{5}$$

Where: t – time [s], for the dynamics of the process, N – number of components, $c_i(r,z,t)$ – concentration of the i-th component in water [mol/m^3 or kg/m^3], $D_{i,\text{eff}}$ – effective diffusion coefficient [m^2/s], $r_{i,\text{bulk}}$ – bulk reaction rate in solution [mol/(m^3·s)], a_s – surpace area of per unit volume [m^2/m^3], $r_{i,\text{surf}}$ – surface loss rate [mol/(m^2·s)]

This equation is called the ADR (advection-diffusion-reaction) equation and shows how the concentration of each harmful substance in water changes: change over time = flow transfer + diffusion - reaction - adsorption. This allows you to calculate the quality of the water exiting the filter.

$$\frac{\partial q_i}{\partial t} = k_{f,i}\left(q_i^*(c) - q_i\right). \tag{6}$$

Where: $q_i(r,z,t)$ – capture quantity in the solid phase [mol/kg], $k_{f,i}$ – LDF(linear driving force) kinetic coefficient [1/s], $q_i^*(\mathbf{c})$ – equilibrium adsorption quantity [mol/kg].

This equation represents the adsorption kinetics (LDF) equation and tells us at what rate harmful substances are absorbed into the filter particles. If the particle is still free, a large amount of harmful substance is absorbed; if saturated, absorption slows down.

$$q_i^*(c) = \frac{q_{i,\max} b_i c_i}{1 + \sum_{j=1}^{N} b_j c_j}. \tag{7}$$

Where: $q_{i,\max}$ – maximum adsorption capacity [mol/kg], b_i – Langmuir affinity coefficient [m^3/mol].

This equation represents the Langmuir isotherm. In this case, due to the limited surface area of the adsorbent, harmful substances compete for space and explain the decrease in the efficiency of the filter over time.

$$r_{i,surf} = \rho_s \frac{\partial q_i}{\partial t}. \tag{8}$$

Where: ρ_s – density of adsorbent particles [kg/m^3].

This equation expresses the rate of surface loss. In this case, the change in adsorption in the solid phase reduces the concentration in the liquid. This links the mechanism of loss of harmful substances to the liquid and solid phase.

The colmatation (optional, particle) equations (9)-(10) defined as follows.

$$\begin{aligned}\frac{\partial (\varepsilon c_p)}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r c_p u_r) + \frac{\partial}{\partial z}(c_p u_z) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon D_p \frac{\partial c_p}{\partial r}\right) + \\ + \frac{\partial}{\partial z}\left(\varepsilon D_p \frac{\partial c_p}{\partial z}\right) - k_{\text{dep}} c_p,\end{aligned} \tag{9}$$

$$\frac{\partial \varepsilon}{\partial t} = -\frac{\nu_{\text{dep}}}{\rho_{\text{dep}}} k_{\text{dep}} c_p. \tag{10}$$

Where: $c_p(r,z,t)$ – concentration of particulate matter in water [kg/m^3], D_p – diffucion coefficient of particles [m^2/s], k_{dep} – depolation coefficient [1/s], ν_{dep} – volume fraction of depolation [–], ρ_{dep} – density of settled particles [kg/m^3].

In this case, large particles (sand, clay) block the pores, thus reducing the filter's permeability. As a result, the flow decreases over time.

Membrane equations (if available below, $G_m \equiv G_{out}$) are:

$$J_v = L_p \left(\Delta P - \sum_{i=1}^{N} \sigma_i \Delta \pi_i\right), \tag{11}$$

$$J_i = (1-\sigma_i)\, c_{i,\text{avg}} J_v - P_{s,i} \Delta c_i, \tag{12}$$

$$-\varepsilon D_{i,eff} \frac{\partial c_i}{\partial n} + c_i J_v = J_i, u_n|_{G_m} = J_v, \tag{13}$$

$$J_v = \frac{\Delta P}{\mu (R_m + R_c)}, R_c = \alpha_c \delta_c, \frac{\partial \delta_c}{\partial t} = \frac{J_v c_{p,m}}{\rho_c}. \tag{14}$$

Here: G_{in} – inlet surface (from above, $z = 0$), G_{out} – outlet surface (from below, $z = H$), J_v – volumetric flow through the membrane (permeat flux) [m/s], L_p – membrane hydraulic permeability [m/(Pa·s)], ΔP – transmembrane pressure difference [Pa], σ_i – reflection coefficient (0–1), π_i – osmotic pressure [Pa], J_i – i-membrane flow of the i-th component [mol/(m^2·s)], $c_{i,\text{avg}}$ – average concentration near the membrane [mol/m^3], $P_{s,i}$ – salt permeability [m/s], $\partial/\partial n$ – normal derivative operator (at the membrane level), R_m – internal membrane resistance [1/m], – cake resistance [1/m], α_c – specific cake resistance [m/kg], $\delta_c(r,z,t)$ – cake thickness [m], $c_{p,m}$ – particle concentration on the membrane [kg/m^3], ρ_c – cake density [kg/m^3].

Boundary conditions are determined as follows: at the inlet, the pressure and composition of the water are given, at the outlet, it is released into the atmosphere. The flow along the side wall and axis does not pass, symmetry is preserved. Special conditions (flow and mass balance) are applied to the membrane surface.

Boundary conditions are given in equations (15)-(19):
Entrance (from top, G_{in}) boundary conditions

$$p = p_{in}, c_i = c_{i,in}(t) \ \ (i = 1, \ldots, N). \tag{15}$$

Exit (from below, G_{out}, $z = H$) boundary conditions

$$p = p_{out} \approx p_{atm}, \ -\varepsilon D_{i,eff} \frac{\partial c_i}{\partial z} + c_i u_z = 0. \tag{16}$$

Boundary conditions of the side wall (G_r, $r = R$)

$$u_r = 0, \frac{\partial u_z}{\partial r} = 0, \frac{\partial c_i}{\partial r} = 0. \tag{17}$$

Boundary conditions for the axis of symmetry (G_0, $r = 0$)

$$u_r = 0, \frac{\partial u_z}{\partial r} = 0, \frac{\partial c_i}{\partial r} = 0. \tag{18}$$

Membrane level (if applicable, G_m) boundary conditions

$$u_n = J_v, -\varepsilon D_{i,eff} \frac{\partial c_i}{\partial n} + c_i J_v = J_i. \tag{19}$$

The initial conditions (in the case $t = 0$) are determined using equations(20)-(23)

$$u_r(r, z, 0) = u_{r,0}(r, z), u_z(r, z, 0) = u_{z,0}(r, z), p(r, z, 0) = p_0(r, z), \tag{20}$$

$$c_i(r, z, 0) = c_{i,0}(r, z), q_i(r, z, 0) = q_{i,0}(r, z) \ (i = 1, \ldots, N), \tag{21}$$

$$\varepsilon(r, z, 0) = \varepsilon_0(r, z), \delta_c(r, z, 0) = 0. \tag{22}$$

Below are the domain of definition of each variable, the division of boundaries, the normal, and the calculation scheme.
Geometry, time, and divisions are defined as follows:
Physical domain

$$\Omega_p = (0, R) \times (0, H) \subset^2_{r,z},$$

time interval

$$t \in (0, T],$$

Boundaries:

$$G_{in} = \{z = 0, 0 \leqslant r \leqslant R\}, \ G_{out} = \{z = H, 0 \leqslant r \leqslant R\},$$
$$G_r = \{r = R, 0 \leqslant z \leqslant H\}, \ G_0 = \{r = 0, 0 \leqslant z \leqslant H\}, \ G_m \equiv G_{out}.$$

Normal direction: outward normal, $u_n = \mathbf{u} \cdot n$.

3 Solution of the problem

When solving the above equations, exact analytical solutions lead to complex calculations and difficulties. Therefore, the results of numerical methods are considered tools for solving these equations. One of the most effective methods for applying numerical solutions is the finite difference method. Determining the solution in this way involves the following steps: Grids and designations are entered as follows:
Spatial nodes – $r_i = i\Delta r, i = 0, \ldots, N_r$; $z_j = j\Delta z, j = 0, \ldots, N_z$.

Time - $t^n = n\Delta t, n = 0, 1, 2, \ldots$.

Discrete fields - $p^n_{i,j}$, $u^n_{r,i,j}$, $u^n_{z,i,j}$.

Concentration for each component - $k = 1, \ldots, N$, concentration - $c^n_{k,i,j}$, adsorption - $q^n_{k,i,j}$.

Partion concentration: $c^n_{p,i,j}$; porosity: $\varepsilon^n_{i,j}$; membrane layer: $\delta^n_{c,i}$ (if present, at $j = N_z$), v – permeability (Kozeny–Carman).

Auxiliary network nodes are entered as follows:

$$r_{i+\frac{1}{2}} = r_i + \frac{\Delta r}{2},\ v.$$

Auxiliary differential operators (central differences) are defined as follows: Central gradient operator diagram

$$(\partial_r \varphi)^n_{i,j} = \frac{\varphi^n_{i+1,j} - \varphi^n_{i-1,j}}{2\Delta r}, (\partial_z \varphi)^n_{i,j} = \frac{\varphi^n_{i,j+1} - \varphi^n_{i,j-1}}{2\Delta z}.$$

Cylindrical Laplace operator diagram

$$(\nabla^2 \varphi)^n_{i,j} = \frac{1}{r_i}\frac{\varphi^n_{i+1,j} - \varphi^n_{i-1,j}}{2\Delta r} + \frac{\varphi^n_{i+1,j} - 2\varphi^n_{i,j} + \varphi^n_{i-1,j}}{\Delta r^2} + \frac{\varphi^n_{i,j+1} - 2\varphi^n_{i,j} + \varphi^n_{i,j-1}}{\Delta z^2}.$$

Divergence operator diagram

$$(\nabla \cdot \mathbf{u})^n_{i,j} = \frac{1}{r_i}\frac{r_{i+\frac{1}{2}} u^n_{r,i+\frac{1}{2},j} - r_{i-\frac{1}{2}} u^n_{r,i-\frac{1}{2},j}}{\Delta r} + \frac{u^n_{z,i,j+\frac{1}{2}} - u^n_{z,i,j-\frac{1}{2}}}{\Delta z},$$

$$u^n_{z,i,j+\frac{1}{2}} = \frac{u^n_{z,i,j+1} + u^n_{z,i,j}}{2}.$$

The discrete Kozeny-Carman formula is introduced as follows:

$$\varkappa^n_{i,j} = \frac{\left(\varepsilon^n_{i,j}\right)^3 d_f^2}{180\left(1 - \varepsilon^n_{i,j}\right)^2}.$$

Equations for hydraulics (Brinkman–Darcy+ projection) are introduced as follows:

"Darcy step" (velocity determination by pressure gradient) discrete values

$$u^{n+\frac{1}{2}}_{r,i,j} = -\frac{\varkappa^n_{i,j}}{\mu}(\partial_r p)^n_{i,j}, u^{n+\frac{1}{2}}_{z,i,j} = -\frac{\varkappa^n_{i,j}}{\mu}(\partial_z p)^n_{i,j}.$$

Brinkman diffusion/resistance correction (explicit) schemes

$$u^{n+1}_{r,i,j} = u^{n+\frac{1}{2}}_{r,i,j} + \Delta t\left[\frac{\mu}{\rho}(\nabla^2 u_r)^n_{i,j} - \frac{\mu}{\rho \varkappa^n_{i,j}} u^n_{r,i,j}\right],$$

$$u^{n+1}_{z,i,j} = u^{n+\frac{1}{2}}_{z,i,j} + \Delta t\left[\frac{\mu}{\rho}(\nabla^2 u_z)^n_{i,j} - \frac{\mu}{\rho \varkappa^n_{i,j}} u^n_{z,i,j}\right]$$

Projection equations (to enhance compression) are introduced as follows.

Determination of pressure renewal in the Poisson operator

$$(\nabla^2 p)^{n+1}_{i,j} = \frac{\rho}{\Delta t}(\nabla \cdot \mathbf{u})^{n+1}_{i,j}.$$

In practice, we can balance the velocity by performing this equation up to 3 times in Jacobi/GS relaxation steps

$$u_{r,i,j}^{n+1} \leftarrow u_{r,i,j}^{n+1} - \frac{\Delta t}{\rho}(\partial_r p)_{i,j}^{n+1}, \;\; u_{z,i,j}^{n+1} \leftarrow u_{z,i,j}^{n+1} - \frac{\Delta t}{\rho}(\partial_z p)_{i,j}^{n+1}.$$

The index range is defined as follows: for internal nodes $i = 1, \ldots, N_r - 1$, $j = 1, \ldots, N_z - 1$. For boundary values, the boundary conditions of Section 5 are applied.

Substance transport (ADR) is introduced for each component as follows:

Upwind convection flow detection schemes:

For the radial direction

$$c_{k,i+\frac{1}{2},j}^{n,\mathrm{up}} = \begin{cases} c_{k,i,j}^n, \;\; u_{r,i+\frac{1}{2},j}^n > 0, \\ c_{k,i+1,j}^n, \;\; u_{r,i+\frac{1}{2},j}^n \leqslant 0, \end{cases} \quad c_{k,i-\frac{1}{2},j}^{n,\mathrm{up}} = \begin{cases} c_{k,i-1,j}^n, \;\; u_{r,i-\frac{1}{2},j}^n > 0, \\ c_{k,i,j}^n, \;\; u_{r,i-\frac{1}{2},j}^n \leqslant 0, \end{cases}$$

$$(\mathcal{C}_r)_{i,j}^n = \frac{1}{r_i} \frac{r_{i+\frac{1}{2}} u_{r,i+\frac{1}{2},j}^n c_{k,i+\frac{1}{2},j}^{n,\mathrm{up}} - r_{i-\frac{1}{2}} u_{r,i-\frac{1}{2},j}^n c_{k,i-\frac{1}{2},j}^{n,\mathrm{up}}}{\Delta r}.$$

For axial direction

$$c_{k,i,j+\frac{1}{2}}^{n,\mathrm{up}} = \begin{cases} c_{k,i,j}^n, \;\; u_{z,i,j+\frac{1}{2}}^n > 0, \\ c_{k,i,j+1}^n, \;\; u_{z,i,j+\frac{1}{2}}^n \leqslant 0, \end{cases} \quad c_{k,i,j-\frac{1}{2}}^{n,\mathrm{up}} = \begin{cases} c_{k,i,j-1}^n, \;\; u_{z,i,j-\frac{1}{2}}^n > 0, \\ c_{k,i,j}^n, \;\; u_{z,i,j-\frac{1}{2}}^n \leqslant 0, \end{cases}$$

$$(\mathcal{C}_z)_{i,j}^n = \frac{u_{z,i,j+\frac{1}{2}}^n c_{k,i,j+\frac{1}{2}}^{n,\mathrm{up}} - u_{z,i,j-\frac{1}{2}}^n c_{k,i,j-\frac{1}{2}}^{n,\mathrm{up}}}{\Delta z}.$$

Schemes for diffusion (central, effective)

$$(\mathcal{D})_{i,j}^n = \frac{1}{r_i} \frac{r_{i+\frac{1}{2}} \varepsilon_{i+\frac{1}{2},j}^n D_{k,eff}^n \left(c_{k,i+1,j}^n - c_{k,i,j}^n\right) - r_{i-\frac{1}{2}} \varepsilon_{i-\frac{1}{2},j}^n D_{k,eff}^n \left(c_{k,i,j}^n - c_{k,i-1,j}^n\right)}{\Delta r^2} + \\ + \varepsilon_{i,j}^n D_{k,eff}^n \frac{c_{k,i,j+1}^n - 2c_{k,i,j}^n + c_{k,i,j-1}^n}{\Delta z^2},$$

where

$$\varepsilon_{i\pm\frac{1}{2},j}^n = \frac{\varepsilon_{i\pm1,j}^n + \varepsilon_{i,j}^n}{2}.$$

Sources (reaction/adsorption) equations in explicit schema

$$R_{k,i,j}^n = -r_{k,\mathrm{bulk},i,j}^n - a_s r_{k,\mathrm{surf},i,j}^n.$$

Conservative form (with pores) schemes

$$W = \varepsilon c_k,$$
$$W_{i,j}^{n+1} = W_{i,j}^n - \Delta t \left[(\mathcal{C}_r)_{i,j}^n + (\mathcal{C}_z)_{i,j}^n\right] + \Delta t (\mathcal{D})_{i,j}^n + \Delta t R_{k,i,j}^n.$$

Updated by $c_{k,i,j}^{n+1} = \frac{W_{i,j}^{n+1}}{\varepsilon_{i,j}^{n+1}}$ (ε^{n+1} determined in the following schemes).

Schemes for adsorption (LDF) and Langmuir isotherm:

Schematic representation for Langmuir equilibrium

$$q_{k,i,j}^{*,n} = \frac{q_{k,\max} b_k c_{k,i,j}^n}{1 + \sum_{m=1}^N b_m c_{m,i,j}^n}.$$

Schematic representation for LDF kinetics (explicit)

$$q_{k,i,j}^{n+1} = q_{k,i,j}^{n} + \Delta t k_{f,k} \left(q_{k,i,j}^{*,n} - q_{k,i,j}^{n} \right).$$

Schematic view for surface source

$$r_{k,\text{surf},i,j}^{n} = \rho_s \frac{q_{k,i,j}^{n+1} - q_{k,i,j}^{n}}{\Delta t}.$$

Schemes for particle clogging and porosity are determined as follows.

ADR schema for particles:

$$(\varepsilon c_p)_{i,j}^{n+1} = (\varepsilon c_p)_{i,j}^{n} - \Delta t \left[(\mathcal{C}_r^{(p)})_{i,j}^{n} + (\mathcal{C}_z^{(p)})_{i,j}^{n} \right] + \Delta t (\mathcal{D}_p)_{i,j}^{n} - \Delta t k_{\text{dep}} c_{p,i,j}^{n}.$$

Where $\left(\mathcal{C}_r^{(p)}\right)$, $\left(\mathcal{C}_z^{(p)}\right)$, $(\mathcal{D}_p)$ is determined by the formulas in part 4 and using c_p and $D_{p,eff}$.

Porosity renewal scheme

$$\varepsilon_{i,j}^{n+1} = \varepsilon_{i,j}^{n} - \Delta t \frac{\nu_{\text{dep}}}{\rho_{\text{dep}}} k_{\text{dep}} c_{p,i,j}^{n},$$

$$\varkappa_{i,j}^{n+1} = \varkappa \left(\varepsilon_{i,j}^{n+1} \right).$$

Determination of the membrane diagram (if it is present $j = N_z$ at the output):

Volumetric flow density diagram

$$J_{v,i}^{n} = \frac{\Delta P}{\mu \left(R_m + R_{c,i}^{n} \right)}, R_{c,i}^{n} = \alpha_c \delta_{c,i}^{n}.$$

Flow balance for each component (for normal $+\hat{z}$)

$$-\varepsilon_{i,N_z}^{n} D_{k,eff}^{n} \frac{c_{k,i,N_z}^{n} - c_{k,i,N_z-1}^{n}}{\Delta z} + c_{k,i,N_z}^{n} J_{v,i}^{n} = J_{k,i}^{n},$$

where $J_{k,i}^{n}$ — the flow of matter through the membrane (depending on your model, for example $J_k = P_k \left(c_{\text{up}} - c_{\text{down}} \right)$).

Colmatation thickness over the membrane

$$\delta_{c,i}^{n+1} = \delta_{c,i}^{n} + \Delta t \frac{J_{v,i}^{n} c_{p,m,i}^{n}}{\rho_c},$$

Where $c_{p,m,i}^{n}$ – concentration of particles on the membrane surface (usually $j = N_z$ or the value of the adjacent cell).

The schemes of boundary and initial conditions are determined as follows:

Initial conditions (for all i, j)

$$p_{i,j}^{0} = p_0 \left(r_i, z_j \right), u_{r,i,j}^{0} = u_{r0} \left(r_i, z_j \right), u_{z,i,j}^{0} = u_{z0} \left(r_i, z_j \right),$$

$$c_{k,i,j}^{0} = c_{k0} \left(r_i, z_j \right), q_{k,i,j}^{0} = q_{k0} \left(r_i, z_j \right),$$
$$c_{p,i,j}^{0} = c_{p0} \left(r_i, z_j \right), \varepsilon_{i,j}^{0} = \varepsilon_0 \left(r_i, z_j \right), \delta_{c,i}^{0} = \delta_{c0} \left(r_i \right).$$

Schemes for inlet $z = 0$ (i.e. $j = 0$)

Pressure and speed condition

$$p_{i,0}^{n} = p_{\text{in}} \left(t^n \right), u_{z,i,\frac{1}{2}}^{n} = u_{\text{in}} \left(t^n \right).$$

Scheme for determining concentrations (according to Dirichlet)

$$c^n_{k,i,0} = c_{k,\text{in}}\left(t^n\right), c^n_{p,i,0} = c_{p,\text{in}}\left(t^n\right).$$

If the velocity is given, the pressure gradient is matched with the central/boundary difference at the input.

Schemes for outlet $z = H$ (i.e. $j = N_z$)

For pressure:

$$p^n_{i,N_z} = p_{\text{out}} \left(\approx p_{\text{atm}}\right).$$

Zero gradient (Neumann) or convective output if there is no membrane:

$$\frac{c^n_{k,i,N_z} - c^n_{k,i,N_z-1}}{\Delta z} = 0 \text{ or } \; -\varepsilon D_{k,eff}\frac{c^n_{k,i,N_z} - c^n_{k,i,N_z-1}}{\Delta z} + c^n_{k,i,N_z} u^n_{z,i,N_z-\frac{1}{2}} = 0.$$

If the membrane is present, the flow balance and refresh δ_c in Part 7 is applied.

Schemes for the side wall $r = R$ (i.e. $i = N_r$)

Diagrams for radial and symmetrical axil directions

$$u^n_{r,N_r,j} = 0, \frac{u^n_{z,N_r,j} - u^n_{z,N_r-1,j}}{\Delta r} = 0.$$

Zero flow for diffusion

$$\frac{c^n_{k,N_r,j} - c^n_{k,N_r-1,j}}{\Delta r} = 0, \;\; \frac{c^n_{p,N_r,j} - c^n_{p,N_r-1,j}}{\Delta r} = 0.$$

On symmetric axes $r = 0$ (i.e. $i = 0$):

$$u^n_{r,0,j} = 0, \frac{u^n_{z,1,j} - u^n_{z,0,j}}{\Delta r} = 0, \;\; \frac{c^n_{k,1,j} - c^n_{k,0,j}}{\Delta r} = 0, \frac{c^n_{p,1,j} - c^n_{p,0,j}}{\Delta r} = 0.$$

Approaches $\partial_{rr}\varphi$ the limit $\frac{1}{r}\partial_r\varphi$ at; in effect

$$\left(\nabla^2\varphi\right)^n_{0,j} \approx \frac{2\left(\varphi^n_{1,j} - \varphi^n_{0,j}\right)}{\Delta r^2} + \frac{\varphi^n_{0,j+1} - 2\varphi^n_{0,j} + \varphi^n_{0,j-1}}{\Delta z^2}.$$

Complete order of the time step (index range) sequence of actions performed: At each time step: (a) $\varkappa^n_{i,j} = \varkappa\left(\varepsilon^n_{i,j}\right)$ is calculated for all of $0 \leqslant i \leqslant N_r, 0 \leqslant j \leqslant N_z$. (b) Darcy step $u^{n+\frac{1}{2}}_{r,i,j}, u^{n+\frac{1}{2}}_{z,i,j}$ is found at

$$i = 1..N_r - 1, j = 1..N_z - 1.$$

(c) Brinkman adjustment: $u^{n+1}_{r,i,j}, u^{n+1}_{z,i,j}$ will be updated explicitly in $i = 1..N_r - 1, j = = 1..N_z - 1$. (d) Projection (for arbitrary 1-3 relexation): $p^{n+1}_{i,j}$ (in internal nodes), then u^{n+1} corrected with a gradient. (e) For each k: $q^{n+1}_{k,i,j}$ will be updated with LDF(all nodes). $(\varepsilon c_k)^{n+1}_{i,j}$ update in internal nodes, then apply to the boundary conditions. If determined $c^{n+1}_{k,i,j} = (\varepsilon c_k)^{n+1}_{i,j}/\varepsilon^{n+1}_{i,j}$is applied. (f) By particle: $(\varepsilon c_p)^{n+1}_{i,j}$ is updated in internal nodes, then applied in boundary conditions

$$\varepsilon^{n+1}_{i,j} = \varepsilon^n_{i,j} - \Delta t\left(\nu_{\text{dep}}/\rho_{\text{dep}}\right) k_{\text{dep}} c^n_{p,i,j}.$$

$\varkappa_{i,j}^{n+1}$ is recalculated. (g) If there is a membrane ($j = N_z$):$J_{v,i}^n$, $J_{k,i}^n$ the flux conditions with and $\delta_{c,i}^{n+1}$ are applied. (h) All boundary conditions are applied as in Section 8. 11) CFL(Courant-Friedrichs-Lewy) condition for stability:

$$\Delta t \leqslant \min\left\{\frac{\Delta r}{\max|u_r|}, \frac{\Delta z}{\max|u_z|}, \frac{1}{2}(D_{eff}^{\max}\left(\frac{1}{\Delta r^2}+\frac{1}{\Delta z^2}\right))^{-1}, \frac{\rho\varkappa_{\min}}{\mu}, \frac{1}{k_{f,\max}}, \frac{\rho_{\text{dep}}}{\nu_{\text{dep}}k_{\text{dep}}c_{p,\max}}\right\}.$$

4 Conclusion

In this study, hydraulic and mass transfer processes occurring in a cylindrical porous filter and membrane system were mathematically modeled. In this case, the pressure and velocity fields of the flow were taken into account using the Brinkman-Darcy equations, and the transport of particulate and dissolved components was described based on the advection-diffusion-reaction (ADR) equations. At the same time, the LDF-kinetics model and the Langmuir isotherm were used for the adsorption process, taking into account the penetration of harmful substances and ions into the solid phase. In addition, the model included colmatation processes and the influence of the cake layer formed at the membrane level on the flow.

Since solving the above equations in exact analytical form is very complex from a practical point of view, a solution based on numerical methods was chosen in this work. In particular, using the finite difference method, spatially and temporally discrete circuits were constructed, and the CFL (Courant-Friedrichs-Lewy) condition was used to ensure their stable operation. With the help of discrete schemes, the main variables, such as pressure, speed, concentration, and adsorbed quantity, were updated over time, and the dynamic development of the process was observed.

As a result of studying the literature, it became known that previously proposed models were often limited to the study of individual processes (for example, only hydraulics or only adsorption). The novelty of this work lies in the fact that all the main processes - fluid movement, transport of substances, adsorption, colmatation, and membrane resistance - are combined into a single mathematical model. As a result, the possibility of a more complete and accurate study of the complex mechanisms of the filtration process has been created.

Sonli results of the numerical calculation showed the basic regularities of the filtration process. In particular, it was found that the flow rate and concentration distribution change significantly over time, the cake layer formed on the membrane sharply reduces permeability, and the overall effectiveness of the colmatation process is directly affected. The obtained results can be used in practical filtration systems for flow control, increasing efficiency, and optimizing filtration time. Also, the developed model can be further improved by comparing it with experimental data, evaluating new adsorbent materials, and adding more complex physicochemical processes.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА ФИЛЬТРОВАНИЯ ЖИДКОГО РАСТВОРА В ЦИЛИНДРИЧЕСКОМ ПОРИСТОМ ФИЛЬТРЕ

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В работе представлена математическая и численная модель процесса фильтрования жидкого раствора в цилиндрическом пористом фильтре. Модель основана на уравнениях Бринкмана–Дарси, которые описывают движение жидкости с учётом пористости и проницаемости фильтрующей среды, связанных соотношением Козени–Кармана. Перенос растворённого вещества описывается системой уравнений адвекции–диффузии–реакции, дополненной кинетикой ЛДФ и изотермой Ленгмюра для адсорбции. В модель включено уравнение кольматации, учитывающее осаждение частиц и уменьшение пористости фильтра во времени. Для численного решения разработан конечно-разностный алгоритм с итерационной коррекцией давления методом сопряжённых градиентов, обеспечивающий устойчивость по критерию Куранта–Фридрихса–Леви. Разработанный подход позволяет исследовать взаимодействие гидродинамических, массообменных и адсорбционных процессов, оценивать эффективность фильтрации и прогнозировать срок службы пористых фильтров в системах очистки жидких растворов.

Ключевые слова: гидродинамика пористых сред, перенос массы, уравнения Бринкмана–Дарси, численная аппроксимация, очистка жидких сред.

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