MATHEMATICAL MODELING OF THE WATER PURIFICATION PROCESS TAKING INTO ACCOUNT THE INVERSE EFFECT OF THE PROCESS CHARACTERISTICS ON THE CHARACTERISTICS OF THE ENVIRONMENT

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Abstract: This paper considers and solves the issues of taking into account the inverse effect of process characteristics (liquid concentration and sediment contamination) on the environment characteristics (porosity, filtration, diffusion, mass transfer, etc.) on the example of liquid purification in magnetic and sorption filters. An algorithm for numerical-asymptotic approximation of the corresponding model problem solution is obtained, which is described by a system of non-linear singularly perturbed differential equations of the type “convection-diffusion-mass transfer”. Appropriate ratios (formulas) are effective for optimizing the water treatment process and increasing the treatment system productivity as a whole (allow to determine the filter protective time, the filter size, etc.) in cases of convective predominance and sorption components of the corresponding process over diffusion and desorption which occurs in the vast majority of filter systems. On this basis, a corresponding computer experiment was conducted, the results of which show the proposed model advantages in comparison with classical.

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1. Introduction

An actual problem in the realm of water supply and drainage is the development of water treatment systems, namely the modeling of these systems [1]-[15]. The work [1] describes the development of a two-dimensional numerical model of the mass transfer process in the filter, which can be used in the calculations of different filter types. The authors [2] describe the use of stochastic approaches in modeling the treatment process, in particular mass service theory and the development of its methods, specifically adapted to the water treatment problems. In the paper [3], the authors constructed a mathematical model of filtration taking into account the processes in the bio plateau filter system in the two-dimensional case. The constructed mathematical model takes into account the physical effects of the dynamic change of porosity and the dependence of the filtration coefficient on the concentration of the contaminant. Methodology [4] for solving the model equations and fitting the model parameters to experimental operating data has been developed and programs are written for a digital computer. The model equations, the solution techniques employed, the parameter fitting procedures, and some typical results are presented. In the work [5], a model for calculating the rational design and operational parameters of the installation with granular filter elements was developed. In research [6] considers different versions of models describing the physicochemical wastewater treatment processes. The analysis of research results conducted in [1]-[13] indicates the presence of complex structure interdependencies of different factors, which determine the filtration processes and filtration through porous media, which were not taken into account in the “traditional” (classical, phenomenological) models of such systems. Taking into account various interactions, as well as various additional factors introduced into the “initial” (basic) model for a deeper study of the process, often leads researchers to the need to build cumbersome and inefficient (in terms of numerical implementation and practical use) mathematical models. However, in many practically important cases in the study of such processes can be approached in terms of modeling various kinds of known perturbations (idealized, averaged, basic) backgrounds.

According to the researches considered above, in work questions are considered and solved the issue of taking into account the inverse effect of process
characteristics (concentrations of liquid and sludge contamination) on the environment characteristics (porosity coefficients, filtration, diffusion, mass transfer, etc.) on the example of liquid purification in magnetic and sorption filters.

2. General problem statement

Consider a layer thick \( L \) (filter), which is placed in the Cartesian coordinate system so that the axis 0\( x \) is perpendicular to its surface, and the origin is at its upper boundary. Impurity articles contamination can pass from one state to another (capture-detachment, sorption-desorption processes) with the concentration of the contaminant affecting the considered layer. The pollution concentration is multicomponent. Appropriate filtering process taking into account the process characteristics feedback (liquid and sludge contamination concentrations) on environmental characteristics (porosity coefficients, filtration, diffusion, mass transfer, etc.) is described by the following system of interconnected differential equations:

\[
\begin{align*}
\frac{\partial (\sigma(\rho)c_i)}{\partial t} + \frac{\partial \rho}{\partial t} + \frac{\partial (vc_i)}{\partial x} &= Di \frac{\partial^2 c_i}{\partial x^2}, \\
\frac{\partial \rho}{\partial t} &= \beta(\rho) \left( \sum_{i=1}^{m} k_i c_i \right) - \alpha(\rho) \rho + D* \frac{\partial^2 \rho}{\partial x^2}, \quad (1) \\
c_i \bigg|_{x=0} &= c_i^* (t), \quad \rho \bigg|_{x=0} = \rho^* (t), \quad \frac{\partial c_i}{\partial x} \bigg|_{x=L} = 0, \quad \frac{\partial \rho}{\partial x} \bigg|_{x=L} = 0, \\
c_i \bigg|_{t=0} &= c_{i*} (x), \quad \rho \bigg|_{t=0} = \rho^* (x), \quad (2) \\
v &= \kappa(\rho) \cdot \text{grad} \, P, \quad (3)
\end{align*}
\]

where \( c_i (x, t) \) – the impurities concentration in the liquid medium which filtered; \( \rho(x, t) \) – impurities concentration precipitated in the filter backfill; \( \beta(\rho) \) – coefficient characterizing the mass volumes of deposition of impurity particles per unit time (\( \beta(\rho) = \beta_0 - \varepsilon \beta_\ast \rho(x, t) \)), \( \alpha(\rho) \) – coefficient characterizing the mass volumes of impurity particles detached from the backfill granules at the same time (\( \alpha(\rho) = \alpha_0 + \varepsilon \alpha_\ast \rho(x, t) \)), \( v \) – filtration rate, \( c_i^* (t) \) – the concentration of impurity particles at the filter input, \( \sigma(\rho) \) – the filter nozzle porosity (\( \sigma_0 \) – the output the nozzle porosity, \( \sigma(\rho) = \sigma_0 - \varepsilon \sigma_\ast \rho(x, t) \)); \( D_i = b_i \varepsilon, D_\ast = b_\ast \varepsilon \beta_0, \beta_\ast, \alpha_0, \alpha_\ast, \sigma_0, b_i, k_i, \varepsilon \) – rigid parameters (they characterize the corresponding coefficients \( \beta(\rho), \alpha(\rho), \sigma(\rho) \)) – soft parameters determined experimentally), \( \varepsilon \) – small parameter, \( i = 1, m \), \( P \) – pressure.
3. Solution algorithm (asymptotics)

The solutions of system (1) under conditions (2) are sought in the asymptotic series form ([11]-[13]):

\[
c_i(x,t) = c_{i,0}(x,t) + \sum_{j=1}^{n} \varepsilon^j c_{i,j}(x,t) + \sum_{j=0}^{n+1} \varepsilon^j U_{i,j} (\xi,t) + R_{ci}(x,t,\varepsilon),
\]

\[
\rho(x,t) = \rho_0(x,t) + \sum_{j=1}^{n} \varepsilon^j \rho_j(x,t) + \sum_{j=0}^{2n+1} \varepsilon^{j/2} P_j (\mu,t) + R_{\rho}(x,t,\varepsilon),
\]

where \(R_{ci}, R_{\rho}\) – residual members, \(c_{i,j}(x,t), \rho_j(x,t)\) \((i = 1,m; j = 0,n)\) – members of the regular asymptote parts, \(U_{i,j} (\xi,t), \tilde{U}_{i,j} (\tilde{\xi},t)\) \((i = 1,m; j = 0,n+1)\), \(P_j (\mu,t), \tilde{P}_j (\tilde{\mu},t)\) \((j = 0,2n+1)\) – boundary layer type functions (corrections at the filtration stream inlet and outlet, respectively), \(\tilde{\xi} = x \cdot \varepsilon^{-1}, \tilde{\mu} = x \cdot \varepsilon^{-1/2}\).

Similarly to [14], after substituting (4) in (1) and applying the standard “equalization procedure”, to find the functions \(c_{i,j}\) and \(\rho_j\) \((j = 0,n)\), we come to the following tasks:

\[
\begin{align*}
\sigma_0 \frac{\partial c_{i,0}}{\partial t} + v \frac{\partial c_{i,0}}{\partial x} + k_i c_i &= 0, \\
\frac{\partial \rho_0}{\partial t} &= \beta_0 \left( \sum_{i=1}^{m} k_i c_{i,0} \right) - \alpha_0 \rho_0, \\
c_{i,0}|_{x=0} &= c^*_i(t), \\
\rho_0|_{x=0} &= \rho^*(t), \\
c_{i,0}|_{t=0} &= c^*_{i,i}(x), \\
\rho_0|_{t=0} &= \rho^*_i(x),
\end{align*}
\]

\[
\begin{align*}
-\sigma_* \rho_{i-1} \frac{\partial c_{i,j}}{\partial t} + v \frac{\partial c_{i,j}}{\partial x} - k_i \sigma_* \frac{\partial \rho_{i-1}}{\partial t} c_{i,j} &= g_{i,j}, \\
\frac{\partial \rho_j}{\partial t} &= -\beta_* \rho_{j-1} \left( \sum_{i=1}^{m} k_i c_{i,j} \right) - \alpha_* \rho_{j-1} \rho_j, \\
c_{i,1}|_{x=0} &= 0, \\
\rho_i|_{x=0} &= 0, \\
\rho_i|_{t=0} &= 0, \\
c_{1,1}|_{t=0} &= 0, \\
\rho_i|_{t=0} &= 0, \\
i = 1,m, j = 1,n.
\end{align*}
\]

As a result of their solution we have

\[
c_{i,0}(x,t) = \begin{cases} 
     c^*_1 \left( t - \frac{\sigma_0 x}{v} \right) \cdot e^{k_{i,x}}, & t \geq \frac{\sigma_0 x}{v}, \\
     c^*_{i,i} \left( x - \frac{vt}{\sigma_0} \right) \cdot e^{k_{i,t}}, & t < \frac{\sigma_0 x}{v},
\end{cases}
\]
\[ \rho_0(x, t) = \beta_0 e^{-\alpha t} \int_0^t \left( \sum_{i=1}^m k_i c_{i,0}(x, \tilde{t}) \right) e^{\alpha \tilde{t}} \, d\tilde{t} + \rho^*(x), \]

\[ c_{i,j}(x, t) = \begin{bmatrix} -\sigma_x e \int_0^x \frac{\lambda_j(\tilde{x}, f(\tilde{x}) + t - f(x)) \, d\tilde{x}}{v} \\ \times \int_0^x g_{i,j}(\tilde{x}, f(\tilde{x}) + t - f(x)) e^{\int_0^\tilde{x} \frac{\lambda_j(\tilde{z}, f(\tilde{z}) + t - f(x)) \, d\tilde{z}}{\rho_{j-1}(\tilde{x}, f(\tilde{x}) + t - f(x))}} \, d\tilde{x}, \ t \geq f(x), \\
-\int_0^x \lambda_j(f^{-1}(\tilde{t} + f(x) - t), \tilde{t}) \, d\tilde{t} \\
-\int_0^t \lambda_j(f^{-1}(\tilde{t} + f(x) - t), \tilde{t}) \, d\tilde{t} \\
\times \int_0^t e^{-\lambda_j(f^{-1}(\tilde{t} + f(x) - t), \tilde{t})} \, d\tilde{t} \\
\times g_{i,j}(f^{-1}(\tilde{t} + f(x) - t), \tilde{t}) \, d\tilde{t}, \ t < f(x), \end{bmatrix} \]

\[ \rho_j(x, t) = -\beta_* e^{-\alpha_* \int_0^t \rho_{j-1}(x, \tilde{t}) \, d\tilde{t}} \int_0^t \rho_{j-1} \left( x, \tilde{t} \right) \left( \sum_{i=1}^2 c_{i,j}(x, \tilde{t}) \right) e^{\alpha_* \int_0^\tilde{t} \rho_{j-1}(x, \tilde{t}) \, d\tilde{t}} \, d\tilde{t}, \]

where \( g_{i,j}(x, t) = b_i \frac{\partial^2 c_{i,j-1}}{\partial x^2} + k_1 \rho_{j-1}, \ \lambda_j(x, t) = -k_i \sigma_* \frac{\partial \rho_{j-1}}{\partial t}. \) Approximate functions values \( f_j(x) \) are by interpolating the array \((x_i, t_i), i = 1, n, \) where \( x_i = \Delta x \cdot i, t_{i+1} = t_i + \Delta x \cdot \sigma_* \rho_{j-1}(x_i, t_i). \) The functions \( U_i = \sum_{j=0}^{n+1} U \varepsilon^j, \)

\[ \tilde{U}_i = \sum_{j=0}^{n+1} \tilde{U}_{i,j} \varepsilon^j, \ (i = 1, 2; j = 0, n + 1), \ P = \sum_{j=0}^{2n+1} P \varepsilon^{j/2}, \ \tilde{P} = \sum_{j=0}^{2n+1} \tilde{P}_j \varepsilon^{j/2} (j = 0, 2n + 1) \] designed to eliminate inconsistencies introduced by the built regular parts \( c_i(x, t) = \sum_{j=0}^{n} c_{i,j} \varepsilon^j, \rho(x, t) = \sum_{j=0}^{n} \rho_j \varepsilon^j \) in points neighborhoods \( x = 0, x = L \) (filtration flow inlet and outlet), that is, ensure that the conditions are met:

\[ \frac{\partial}{\partial x} (c + U) = O(\varepsilon^{n+1}), \frac{\partial}{\partial x} (c + \tilde{U}) = O(\varepsilon^{n+1}), \frac{\partial}{\partial x} (\rho + P) = O(\varepsilon^{n+1}), \frac{\partial}{\partial x} (\rho + \tilde{P}) = O(\varepsilon^{n+1}). \] These functions are similar to [13]. To estimate the residual members, we have a corresponding problem similar to [13].
4. Numerical calculations

4.1. Magnetic filter

Consider the purification process of liquid media from ferromagnetic impurities in magnetized porous nozzles, which is one of the most important tasks of removing impurities from corrosion products due to continuous corrosion of process equipment. Impurity particles of media under the action of magnetic force factor $F_c = H \cdot \text{grad}H$ are deposited at the contact points of the nozzles granules, where dimension $F_c$ can reach the value of the order $2 \cdot 10^{15} A^2/m^3$ ($H$ – magnetic field strength). At the initial time ($t = 0$) the porous nozzle is relatively “clean”, that is, not saturated with impurity particles, its porosity – $\sigma_0$. In the process of deposition of impurities, the amount of porosity $\sigma$ gradually decreases, the coefficient of hydraulic resistance increases and accordingly in the system closure case, the magnitude of the pressure drops increases $\Delta P$ in a porous nozzle. The cleaning process efficiency remains at a fairly high level for some time $t = \tau_3$ (filter cycle time, filter protection time). With the accumulation of a critical impurities mass in the volume of the porous nozzle, characterized by the value of the working absorption capacity, the cleaning process efficiency $\psi$, equal to the ratio of the difference between the concentrations of impurities at the filter inlet and outlet to the concentration at the inlet, decreases and the purification mode goes into a non-stationary stage (Fig. 1). As is known [13], when $t > \tau_3$ a certain impurities amount is still deposited in the porous layers of the nozzle, and most of them are “broken” and removed with the cleaned medium. Gradually cells on length of a porous nozzle are as much as possible saturated with impurity and are self-disconnected, at achievement of sometime $\tau_n$ and the cleaning efficiency is reduced to zero.

The impurities magnetic deposition process, which is realized in a magnetic filter ($0 \leq x \leq L$) with a homogeneous granular filter nozzle, is carried out according to the laws, the prototype of which is a classical model of filtration [12], taking into account the inverse effect of the deposited particles on the porosity $\sigma$ and coefficient $\alpha$, as well as the filtration coefficient, [12].

$$\begin{align*}
\frac{\partial (\sigma \rho c(x,t))}{\partial t} + \frac{\partial \rho (x,t)}{\partial t} + v \frac{\partial c(x,t)}{\partial x} &= 0, \\
\frac{\partial \rho (x,t)}{\partial t} &= \beta c (x,t) - \varepsilon \alpha (\rho) \rho (x,t),
\end{align*}$$

(10)

$$\begin{align*}
c|_{x=0} &= c_*(t), \\
c|_{t=0} &= 0, \\
\rho|_{x=0} &= 0, \\
\rho|_{t=0} &= 0,
\end{align*}$$

(11)

$$v = \kappa (\rho) \cdot \text{grad} P,$$
where $\alpha (\rho)$ – coefficient characterizing the mass volumes of impurity particles detached from the nozzle granules at the same time; $\alpha (\rho) = \alpha_0 + \varepsilon \alpha_* \rho (x, t)$, $v$ – filtration rate ($v = \text{const}$, which characterizes the closedness of the technological process), $\sigma (x, t)$ – the filter nozzle porosity ($\sigma_0$ – the initial porosity of the nozzle), $\sigma (x, t) = \sigma_0 - \varepsilon \sigma_* \rho (x, t)$ $\kappa (\rho)$ – filtering factor, $\rho$ – maximum sludge loading, $\kappa (\rho) = \begin{cases} \kappa_0 - \varepsilon \gamma \rho (x, t), & \rho < \rho_{cr} \ (t < \tau_{cr}), \\ \kappa^0, & \rho = \rho_{cr} \ (t \geq \tau_{cr}) \end{cases}$, $\kappa^0 = \kappa_0 - \varepsilon \gamma \rho, \alpha_0, \alpha_*, \sigma_*, \kappa_0, \gamma, \varepsilon$ – rigid parameters (they characterize the corresponding coefficients $\alpha (\rho), \sigma (x, t), \kappa (x, t)$ – soft parameters determined experimentally), $P$ – pressure. This nature of the change in porosity and the coefficient of detached particles is explained by the fact that with increasing impurity particles in the nozzle, the corresponding filtering parameters change. Since the system is closed, a change in the filtration coefficient leads to a change in the pressure drop dimension $\Delta P = P (L, t) - P (0, t)$ in a porous nozzle. The solution of system (7) under conditions (8) is similar to (1) - (2) in the form of asymptotic series (4) (see [9], [11]), Fig. 2.

According to [13] the coefficients of trapped impurity particles and detached particles of sludge are calculated by the following formula: $\beta = \frac{\beta_0 H^{0.75}}{v d^2}$ [13], where $\beta_0$ – free option, $H$ – magnetic field strength, $v$ – filtration rate, $d$ – the granular filter nozzle diameter.

We give the results of calculations by formulas (3) for $c_* (t) = 2 mg/l$, $v = 200 m/h, L = 1 m, \beta_0 = 0.7 \cdot 10^{-9} c^{-1}, \alpha_0 = 0.35 c^{-1}, H = 60 kA/m$, $d = 2.4 mm, \alpha_* = 1$. Fig. 2 shows the distribution of the impurity’s concentration in the liquid and sediment at certain points in time. Hence, setting the output of the filter (at $L = 1$) permissible concentration value $c = c_{cr} = 0.59 \ mg/l$,
find the time of its protective action: \( t = \tau_3 = 71 \text{ hours} \), which differs by 4 hours from the data obtained experimentally [8]. The filter will accumulate 240 g of sediment. We emphasize that in the process of calculation we accepted \( v = \text{const} \), although the filtration coefficient (as well as porosity) decreases due to adhesion to the walls (backfill) of solid particles. This makes it possible to find a filter in each cross section (in every point \( x \), \( 0 \leq x \leq L \)) pressure gradient (pressure), in particular using the formula \( \text{grad } P = v/\kappa (\rho) \) can find the time of receipt of a larger than critical value of the gradient and make appropriate “automation decisions”. The change \( \text{grad } P \) over time is shown in Fig. 3.a.

As seen in Fig. 3.b, in the case \( c_* (t) = c_* = \text{const} \) the filter efficiency does not change until the time moment \( \tau \), after which it begins to decline, which confirms the known fact of the distribution of the filter efficiency over time.

4.2. Sorption filter

The filtration process on sorption filters does not require a closed system, so the filtration rate is not a constant value and, as a rule, the rate changes along the filter over time. To simplify the calculations, we will assume that the concentration of pollution is one-component. It is also necessary to take into account the inverse effect on the porosity and coefficients that characterize the deposition of dirt particles and detachment of sediment particles [9] and longitudinal diffusion. Based on the above, the system (1) - (2) will be rewritten as:

\[
\begin{align*}
\frac{\partial (\sigma(x,t)c(x,t))}{\partial t} + \frac{\partial \rho(x,t)}{\partial t} + \frac{\partial (v(x,t)c(x,t))}{\partial x} &= D \frac{\partial^2 c}{\partial x^2}, \\
\frac{\partial \rho(x,t)}{\partial t} &= \beta (\rho) c(x,t) - \varepsilon \alpha (\rho) \rho(x,t) + D_* \frac{\partial^2 \rho}{\partial x^2},
\end{align*}
\]

(12)
The solutions of system (9) under conditions (10) are sought similarly to the general problem in the form of asymptotic series (see [8], [11]). We give the calculation results by formulas (4) for $c^*_t = 170 \, \text{mg/l}$, $L = 0.8 \, \text{m}$, $\beta_0 = 0.3 \, \text{s}^{-1}$, $\alpha_0 = 0.0056 \, \text{s}^{-1}$, $\sigma_0 = 0.5$, $\alpha_\ast = 1$, $\beta_\ast = 1$, $\sigma_\ast = 1$, $b = b_\ast = 1$, $\varepsilon = 0.001$.

Fig. 4.a and Fig. 4.b illustrate the comparative characteristics of the data obtained experimentally and calculated by the classical Mintz model [8] and calculated by formulas (7), therefore, the calculations result by formulas (7) give greater accuracy than the calculations by the formulas of the classical Mintz model. Also, the received calculation formulas give the ability to calculate dynamics of the concentration advance of pollution and a deposit along the filter (see Fig. 5.a and Fig. 5.b).

5. Conclusions

The paper constructs a mathematical model that takes into account the inverse effect of process characteristics (liquid and sediment pollution concentrations) on environmental characteristics (porosity, filtration, diffusion, mass transfer, etc.) on the example of liquid purification in magnetic and sorption filters, namely:

- the constructed mathematical model is transferred to the process that describes the laws of magnetic deposition of impurities in the porous filter nozzle, the laws of accumulation (“drift”) of impurities in the nozzle, and takes into
Figure 4: a. Impurity concentration distribution at the filter output during the protective action time: 1 - according to the Mintz model; 2 - according to formulas (7), when $d = 0.78 \text{ mm}$, $v = 10 \text{ m/h}$, $\tau_{\text{exp}} = 26.1 \text{ h}$, $\tau_p = 32 \text{ h}$, $\tau_M = 38 \text{ h}$.

b. Impurity concentration distribution at the filter output during the protective action time: 1 - according to the Mintz model; 2 - according to formulas (7), when $d = 0.78 \text{ mm}$, $v = 9 \text{ m/h}$, $\tau_{\text{exp}} = 30.3 \text{ h}$, $\tau_p = 33 \text{ h}$, $\tau_M = 45 \text{ h}$.

Figure 5: a. Impurity concentration distribution along the filter at time $t = 26 \text{ h}$: 1 - according to the Mintz model; 2 - according to formulas (7), when $d = 0.78 \text{ mm}$, $v = 10 \text{ m/h}$.

b. Sludge concentration distribution along the filter at time $t = 26 \text{ h}$: 1 - according to the Mintz model; 2 - according to formulas (7), when $d = 0.78 \text{ mm}$, $v = 10 \text{ m/h}$.
account the inverse effect of sludge concentration on porosity, filtration and mass transfer. An algorithm for solving the corresponding problem is proposed, which, in particular, includes: determination of time \( \tau \) filter nozzle protective action, the limit value determination of the pressure drop \( \Delta P \) and determination \( \text{grad } P \) when change \( x \in [0, L] \) and \( t \in [0, \tau] \). The calculations result of distribution of impurity and mass volume concentration of filtering porous nozzle impurity on height for various moments of time, size of filtering factor at various values of length of a nozzle \( L \) corresponding to time of protective action (filter cycle) of a nozzle are resulted. In this model the process automated control possibility of effective deposition of impurities in the magnetized filter nozzle depending on the initial data of the purified aqueous medium is provided;

- the developed mathematical model is transferred to the process of wastewater treatment on sorption filters taking into account the inverse effect of sludge concentration on the environment characteristics and the variable filtration rate. The calculations result of the impurity concentration distribution and mass volume of impurities on the height of the filter porous nozzle for different times, the value of the filtration coefficient at different values of the filtration rate, and the characteristics of the filter backfill. A comparative description of the data obtained experimentally and calculated on the basis of the classical Mintz model and the formulas obtained by us (in particular, according to the data shown in Fig. 4.a and Fig. 4.b, we see that the accuracy of calculations according to our proposed formulas is much higher compared to the calculations obtained by the classical Mintz model).

References


