Computer Prediction of Adsorption Water Purification Process in Rapid Cone-Shaped Filters

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Abstract— In the paper a mathematical model for computer predicting the process of adsorption purification of water from impurities in rapid filters taking into account changes in the temperature of the filtration flow along the height of the filter while observing the constant filtration rate is formulated. An algorithm for numerically-asymptotic approximation of solution of the corresponding nonlinear singularly perturbed boundary value problem for a model region of a conical shape, bounded two equipotential surfaces and a surface flow, is developed. The proposed model allows through computer experiments to investigate changes in the characteristics of porous loads (filtration coefficients, active porosity), to predict the optimal variants for using adsorbents, and increasing the duration of the filters operation due to the choice of their shape, taking into account the effect on the process of adsorption purification of water not only changes in the filtration rate flow along the height of the filter, but also the temperature.

Keywords— mathematical model, computer prediction, process of water purification, impurity, adsorption, temperature, rapid filter, cone-shaped form, homogeneous porous load.

I. INTRODUCTION

Quick filters or columns for the adsorption purification of drinking water are usually used in the final stage of water treatment, when from it by gravity sedimentation, filtration, coagulation most of the impurities have been removed [1, 2]. The principle of fast filters is based on pressure filtration of water through a layer of granular material – adsorbent, which serves to remove both mechanical impurities due to the forces of adhesion-suppression and inertial interaction, and dissolved impurities due to adsorption. As adsorbents, natural (bentonite, montmorillonite, peat), artificial (activated carbon, artificial zeolites, polysorbents) and synthetic materials (nanostructured carbon sorbents) are used [3]. Continuous adjustment of the filter speed is the basis for achieving optimum technological mode of operation of filters. Maintaining a constant set filtering speed can only be achieved through automatic adjustment.

Continuous filtration speed is achieved by increasing the opening increasing of the filtrate pipelines latch as the filter loading resistance increases due to the accumulation of impurity particles in it. When the latch is fully open, the filter is switched off from the flushing operation. The impulse to increase the opening of the latch on the filtrate pipeline is to change the water level on the filter (controlled by the float device) or the flow rate of water in the filtrate pipeline (controlled by a throttling device and a diffmanometer). [4].

The ever-increasing needs of the economy for purified water and the rising cost of filter materials require research to optimize the use of adsorbents and increase the life of filters by choosing their form, in particular, taking into account the influence on the process of adsorption purification of water changes in the temperature of the filtration flow along the height of the filter.

The speed of the adsorption process depends on the concentration, nature and structure of the impurities, the filtration rate and the temperature of the filtration flow, the type and properties of the adsorbent [5]. Adsorption - the process is reversible, ie the adsorbed impurity (adsorbate) can pass from the adsorbent back into the filtration stream. Increasing the temperature promotes desorption, resulting in a reduced amount of adsorbed impurity. Under other equal conditions the flow rates of forward (sorption) and reverse (desorption) processes are proportional to the concentration of impurities in the filtration stream and on the surface of the adsorbent grains.

According to literature sources, in particular [6 – 13], many domestic and foreign scientists have made a significant contribution to the development of the theoretical foundations for the purification of impurities by filtration through porous loading. It should be noted that as a mathematical model of the process of liquid purification from impurities by domestic researchers, the model of D.M. Mintz [7] is most often used at a constant speed of filtering and temperature, or some of its modification (an improved model). In [14], its spatial
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generalization is proposed to predict the process of water purification from impurities in fast cone-shaped filters while maintaining a constant filtration rate. The model proposed in this work is more efficient for theoretical studies aimed at optimizing the filtering process parameters (duration, shape, filter size, layer height, etc.) by introducing additional equations to determine the change in active porosity and filtration coefficient of filter loading along its height, taking into account diffusion in the filtration stream and on the surface of the loading grains. An urgent task is to generalize the appropriate model for computer-based forecasting of the process of adsorption purification of water from impurities in fast filters. It is necessary to take into account changes in the temperature of the filtration stream along the height of the filter while maintaining a constant filtration rate. This will allow, due to the computer experiments, to predict the optimal use of adsorbents and increase the life of filters by choosing their shape, taking into account not only the change in filtration flow along the filter height, but also the temperature.

II. MATHEMATICAL MODEL

We simulate the process of adsorption purification of water from impurities in a fast cone-shaped filter – a spatial one-connected region \( G_z (z = (x, y, z)) \), bounded by smooth, orthogonal interconnecting lines, by two equipotential surfaces \( S_\alpha, S^* \) and by the flow surface \( S^{**} \) (Fig. 1a). We assume that the convective components of mass transfer and adsorption outweigh the contribution of diffusion and desorption. In addition, the impact of temperature effects on the internal kinetics of mass transfer is taken into account due to changes in the filtration flow temperature due to adsorption and desorption processes. So for the region \( G = G_z \times (0, \infty) \) the corresponding spatial modeling problem, taking into account the reverse influence of process characteristics (impurity concentration, respectively, in the filtration flow and on the surface of the adsorbent, the temperature) on the loading characteristics (filtration coefficients, porosity, adsorption, desorption) will consist of the equations of motion of the filtration stream (according to Darcy’s law) and balance of mass and heat:

\[
\vec{v} = \kappa_0 \cdot \text{grad} \, \varphi, \; \text{div} \, \vec{v} = 0, \quad (1)
\]

\[
(\sigma \cdot C)_{t} = \text{div} (D \cdot \text{grad} \, C) - \vec{v} \cdot \text{grad} \, C - \alpha \cdot C + \beta \cdot U, \\
(\sigma \cdot U)_{t} = \text{div} (D^s \cdot \text{grad} \, U) + \alpha \cdot C - \beta \cdot U, \\
(\sigma \cdot T)_{t} = \text{div} (D^{**} \cdot \text{grad} \, T) - \vec{v} \cdot \text{grad} \, T + \\
\gamma \cdot (\alpha \cdot C - \beta \cdot U), \quad \kappa' = -\mu \cdot U, \quad \sigma'_s = -\lambda \cdot U \quad (2)
\]

and are supplemented by the following boundary conditions:

\[
[\varphi]_{S_\alpha} = \varphi_\alpha, \; \varphi'_s |_{S^{**}} = 0, \quad (3)
\]

\[
[C]_{S_\alpha} = c^*, \; C'_s |_{S^{**}} = 0, \quad C'_s |_{S^{**}} = 0, \quad (4)
\]

\[
[U]_{S_\alpha} = u^*, \; U'_s |_{S^{**}} = 0, \quad U'_s |_{S^{**}} = 0, \quad (4)
\]

\[
[T]_{S_\alpha} = T^*, \; T'_s |_{S^{**}} = 0, \quad T'_s |_{S^{**}} = 0, \quad (4)
\]

and initial conditions:

\[
\begin{align*}
C_{|_{t=0}} &= c_0^*, \quad U_{|_{t=0}} = u_0^*, \quad T_{|_{t=0}} = T_0^*, \\
\kappa_{|_{t=0}} &= \kappa_0^*, \quad \sigma'_s |_{t=0} = 0
\end{align*}
\quad (5)
\]

where \( \varphi = \varphi(x, y, z) \) and \( \vec{v} = \vec{v}(v_x, v_y, v_z) \) – respectively the potential and the velocity vector of the filtratio, \( 0 \leq \varphi_x < \varphi < \varphi^* < \infty, \)

\[
v = \sqrt{v_x^2(x, y, z) + v_y^2(x, y, z) + v_z^2(x, y, z)} \geq 0, \quad \kappa_0^* - \text{initial filtration coefficient, } \kappa_0^* > 0, \quad \vec{n} \rightarrow \text{outer normal to the corresponding surface, } C = C(x, y, z, t) \text{ i.e. } U = U(x, y, z, t) \rightarrow \text{the concentration of impurities, respectively, in the filtration flow and on the surface of the adsorbent loading, } T = T(x, y, z, t) \rightarrow \text{the temperature of the filtration flow at a point } (x, y, z) \text{ at time } t, \quad \kappa = \kappa(x, y, z, t) \rightarrow \text{filtration coefficient, } \sigma = \sigma(x, y, z, t) \rightarrow \text{active porosity, } D \text{ i } D^* \rightarrow \text{impurity diffusion coefficients, respectively, in the filtration stream and on the surface of the adsorbent, } D = \varepsilon \cdot d_0, \; d_0 > 0, \; D^* = \varepsilon \cdot d_0^*, \; d_0^* > 0, \; D^{**} \rightarrow \text{coefficient of thermal conductivity of the filtration stream, } \sigma^0 = \sigma(x, y, z, t) \rightarrow \text{active porosity, } \alpha \text{ i } \beta \rightarrow \text{coefficients characterizing respectively the volumes of impurities adsorbed from the filtration stream on the surface of the adsorbent and desorbed from the surface of the adsorbent loading into the filtration stream per unit time, }
\]

\[
\begin{align*}
\alpha &= \sum_{s=0}^{2} \sum_{s_1=0}^{2} \sum_{s_2=0}^{2} (\varepsilon + \sigma^0) \beta_{s_1, s_2} \cdot v^{s_1} \cdot T^{s_2}, \quad \beta_{s_1, s_2} \in \mathbb{R} \quad (s_1 = 0, 2, s_2 = 0, 2 - s_1), \\
\beta &= \beta \cdot \gamma, \quad \beta \in \mathbb{R}, \quad \gamma \rightarrow \text{coefficient characterizing the rate of change of filtration flow temperature due to adsorption and desorption processes, } \gamma = \varepsilon \cdot \sigma, \quad \mu \rightarrow \text{coefficients characterizing, respectively, the rate of change of the filter coefficient and the active porosity of the load due to the adsorption of impurities, } \\
\mu &= \varepsilon \cdot \gamma, \quad \beta = \sum_{s=0}^{2} \sum_{s_1=0}^{2} \sum_{s_2=0}^{2} (\varepsilon + \sigma^0) \beta_{s_1, s_2} \cdot v^{s_1} \cdot T^{s_2}, \quad \beta_{s_1, s_2} \in \mathbb{R} \quad (s_1 = 0, 2, s_2 = 0, 2 - s_1), \quad \gamma \rightarrow \text{coefficient characterizing the rate of change of filtration flow temperature due to adsorption and desorption processes, } \gamma = \varepsilon \cdot \sigma, \; \mu \rightarrow \text{coefficients characterizing, respectively, the rate of change of the filter coefficient and the active porosity of the load due to the adsorption of impurities, } \\
\mu &= \varepsilon \cdot \gamma, \quad \beta = \sum_{s=0}^{2} \sum_{s_1=0}^{2} \sum_{s_2=0}^{2} (\varepsilon + \sigma^0) \beta_{s_1, s_2} \cdot v^{s_1} \cdot T^{s_2}, \quad \beta_{s_1, s_2} \in \mathbb{R} \quad (s_1 = 0, 2, s_2 = 0, 2 - s_1), \quad \gamma \rightarrow \text{coefficient characterizing the rate of change of filtration flow temperature due to adsorption and desorption processes, } \gamma = \varepsilon \cdot \sigma, \; \mu \rightarrow \text{coefficients characterizing, respectively, the rate of change of the filter coefficient and the active porosity of the load due to the adsorption of impurities, } \\
\mu &= \varepsilon \cdot \gamma, \quad \beta = \sum_{s=0}^{2} \sum_{s_1=0}^{2} \sum_{s_2=0}^{2} (\varepsilon + \sigma^0) \beta_{s_1, s_2} \cdot v^{s_1} \cdot T^{s_2}, \quad \beta_{s_1, s_2} \in \mathbb{R} \quad (s_1 = 0, 2, s_2 = 0, 2 - s_1), \quad \gamma \rightarrow \text{coefficient characterizing the rate of change of filtration flow temperature due to adsorption and desorption processes, } \gamma = \varepsilon \cdot \sigma, \; \mu \rightarrow \text{coefficients characterizing, respectively, the rate of change of the filter coefficient and the active porosity of the load due to the adsorption of impurities, }
\end{align*}
\]

Similarly [14] by fixing on the surface of a point \( A (A = B) \) and sequential execution of conditional sections \( \Gamma_1 = ALMDBLMC \) i.e. \( \Gamma_2 = ADDA_BCCB, B_{n0} \) along the corresponding surfaces of the flow (we denote for convenience \( \Gamma = \Gamma_1 \cup \Gamma_2 \) problem (1) - (5) is reduced to the solution in the received one-connected region \( G_z \ \Gamma \rightarrow \text{curvilinear parallelepiped } ABCDA_BCCB, \) bounded by two equipotential

...
surfaces $ABB_xA_x$, $CDD_xC_x$ and four flow surfaces $ABCD = ALMD \cup BLMC \cup ABCD \cup ADD_xA_x \cup BCC_xB_x$, which are smooth and orthogonal to each other at angular points and along the edges, with the addition of the impermeability condition $\varphi|_\Gamma = 0$ along the section $\Gamma$ of the problem, described by systems of equations (1), (2) with the following boundary conditions:

$$
\begin{align*}
\varphi|_{ABB_xA_x} &= \varphi_x, & \varphi|_{CDD_xC_x} &= \varphi^*, \\
\varphi|_{ABCD \cup ABCD \cup ADD_xA_x \cup BCC_xB_x} &= 0, \\
C|_{ABB_xA_x} &= c^*_x, & C|_{CDD_xC_x} &= 0, \\
C|_{ADD_xA_x \cup BCC_xB_x \cup ABCD \cup ABCD} &= 0, \\
U|_{ABB_xA_x} &= u^*_x, & U|_{CDD_xC_x} &= 0, \\
U|_{ADD_xA_x \cup BCC_xB_x \cup ABCD \cup ABCD} &= 0, \\
T|_{ABB_xA_x} &= T^*_x, & T|_{CDD_xC_x} &= 0, \\
T|_{ADD_xA_x \cup BCC_xB_x \cup ABCD \cup ABCD} &= 0.
\end{align*}
$$

(6)

initial conditions (5) and subsequent “bonding” of the shores of the conditional section $\Gamma$ using the terms:

$$
\begin{align*}
\varphi|_{ALMD} &= \varphi|_{BLMC} \cdot \varphi|_{ALMD} = \varphi|_{BLMC}, \\
\varphi|_{ADD_xA_x} &= \varphi|_{BCC_xB_x} \cdot \varphi|_{ADD_xA_x} = \varphi|_{BCC_xB_x},
\end{align*}
$$

(8)

and the consistency of the impurity concentrations in the filtration flow and on the surface of the adsorbent loading and the temperature values on the conditional surfaces of the section using the conditions:

$$
\begin{align*}
C|_{ALMD} &= C|_{BLMC} \cdot C|_{ALMD} = C|_{BLMC}, \\
C|_{ADD_xA_x} &= C|_{BCC_xB_x} \cdot C|_{ADD_xA_x} = C|_{BCC_xB_x}, \\
U|_{ALMD} &= U|_{BLMC} \cdot U|_{ALMD} = U|_{BLMC}, \\
U|_{ADD_xA_x} &= U|_{BCC_xB_x} \cdot U|_{ADD_xA_x} = U|_{BCC_xB_x}, \\
T|_{ALMD} &= T|_{BLMC} \cdot T|_{ALMD} = T|_{BLMC}, \\
T|_{ADD_xA_x} &= T|_{BCC_xB_x}, & T|_{ADD_xA_x} &= T^*_x|_{BCC_xB_x}.
\end{align*}
$$

(9)

Similarly [9] by entering a pair of functions $\psi = \psi(x, y, z)$, $\eta = \eta(x, y, z)$ (spatially complex conjugated with function $\varphi(x, y, z)$) such that $\kappa_0^{\varphi} \nabla \varphi = \nabla \varphi \times \nabla \eta$ [16] and replacing the last four of the boundary conditions (6) by the conditions:

$$
\begin{align*}
\varphi|_{ADD_xA_x} &= 0, & \psi|_{BCC_xB_x} &= Q_x, & \eta|_{ABCD} &= 0, \\
\eta|_{ABCD \cup ABCD} &= Q^*, & \text{problem (1), (6), (8) is replaced by the more general direct problem of finding a spatial analogue of the conformal mapping of the one-connected region $G_\nu \cap \Gamma$ to the corresponding region of complex potential – rectangular parallelepiped $G_\nu = A'B'C'D'A'B'C'D'$, where $G_\nu = \{w = (\varphi, \psi, \eta) : \varphi_x < \varphi < \varphi^*, \ 0 < \psi < Q_x, \ 0 < \eta < Q^* \}$, $Q_x, \ Q^*$ – unknown parameters, $Q = Q_x \cdot Q^*$ – complete filtration flow. The algorithm for solving this problem was obtained in [17], in particular, the velocity field $\nu$ was found, parameters $Q_x, Q^*$ and a number of other dimensions.}
\end{align*}
$$

(10)}
\[ \begin{align*}
\tilde{a}_s^* (\phi, \psi, \eta, t) &= \tilde{a}_0^s (\phi, \psi, \eta), \\
\tilde{T}_s^* (\phi, \psi, \eta, t) &= \tilde{T}_0^s (\phi, \psi, \eta, t), \\
\tilde{T}_0^s (\phi, \psi, \eta, t) &= 0,
\end{align*} \]

III. PROBLEM SOLVING AND CONCLUSIONS

Provided that the convective components of heat and mass transfer and adsorption predominate over the contribution of diffusion and desorption, the algorithm for numerically asymptotic approximation of the solution of the corresponding nonlinear singularly perturbed boundary value problem for the model region of cone-shaped bounded by two equipotential surfaces and the surface of the flow, is obtained similarly [14].

The proposed model for a predetermined constant filtration rate allows, by computer experiments, to predict the change in the characteristics of piecewise homogeneous porous loads (filtration coefficients and active porosity), to determine the most optimal use of adsorbents, increase the duration of the filters by choosing their shape, taking into account not only the change in filtration flow rate along the filter height but also the temperature.

REFERENCES

[1] Edzwald J. Water Quality & Treatment. A Handbook on Drinking Water. – McGraw-Hill Professional, 2010. – 1996 p.
[2] Hendricks D. W. Fundamentals of water treatment unit processes: physical, chemical, and biological. – Boca Raton : CRC Press, 2011. – 883 p.
[3] Sakalova H. V., Vasylanych T. M. Doslidzhennya efektyvnosti ochysshennya stichnyx vod vid ioniv vazhkyx metaliv z vykorystannymy priorydnym adsorbutiv: monohrafiya. – Vinnyycya: TOV «Tvory», 2019. – 92 p.
[4] Nezhorova A. B. Osnovy avtomatizacii sistem vodosnabzheniia i vodootvedeniia: Posobie. – Gomel: UO «BelGUT», 2005. – 115 p.
[5] Makarevich N. A., Bogdanovich N. I. Teoreticheskie osnovy adsorbcii: uchebnoe posobie. – Arhangelsk: SAFU, 2015. – 362 p.
[6] Bomba A. Ya., Sazonov A. P. Modelyuvannya nelinijnog-zburnykh processiv ochysshennya ridyn vid bahatokomponentnych zabrudnen’: monohrafiya. – Rivne: NUVHP, 2017. – 296 p.
[7] Minc D. M. Teoreticheskie osnovy tehnologii ochistki vody. – M. : Strojizdat, 1964. – 156 p.
[8] Bomba A. Ya., Prysyazhnyuk I. M., Prysyazhnyuk O. V. Metody teoretyi zburen’ prohnozuvannya procesiv teplomasoperezennya v porystym ta mikroporystym nerezovyslahyv. – Rivne: O. Zen, 2017. – 291 p.