Research Article

Nonlinear Inverse Problem for an Ion-Exchange Filter Model: Numerical Recovery of Parameters

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This paper considers the problem of identifying unknown parameters for a mathematical model of an ion-exchange filter via measurement at the outlet of the filter. The proposed mathematical model consists of a material balance equation, an equation describing the kinetics of ion-exchange for the nonequilibrium case, and an equation for the ion-exchange isotherm. The material balance equation includes a nonlinear term that depends on the kinetics of ion-exchange and several parameters. First, a numerical solution of the direct problem, the calculation of the impurities concentration at the outlet of the filter, is provided. Then, the inverse problem, finding the parameters of the ion-exchange process in nonequilibrium conditions, is formulated. A method for determining the approximate values of these parameters from the impurities concentration measured at the outlet of the filter is proposed.

1. Introduction and Background

One of the key technologies for the preparation of water at thermal power plants and nuclear power plants is the use of ion-exchange materials. Water treatment using ion-exchange methods is based on the passing of source water through a filter bed of ion-exchange material. That material is substantially insoluble in water but capable of ion-exchange with ions contained in the treated water. Water is a good solvent of various salts that have a negative solubility coefficient; that is, when the water temperature rises, the amount of dissolved salts is reduced, and the excess amounts of these salts are precipitated in heated tubes, forming scale with a very low coefficient of thermal conductivity. Power-generating units of thermal power plants (TPP) operate under severely corrosive conditions: high temperature (515–530°C) and pressure (15 MPa) hot steam [1–3]. The main reason for failures of power equipment is failure of the most thermally loaded parts, namely, pipes in which the coolant water flows. Scale restricts flow of heat energy to the coolant (water) and does not allow for the cooling of pipe surfaces; this

causes the surface metal temperature to increase, reaching the critical melting point. The result is an emergency stop of the boiler [3]. Another problem is that the rate of corrosion of the metal under scale on the surface of the tubes sharply increases; that is, scale is a corrosion catalyst [4–7]. Reducing metal corrosion requires not only using materials with high corrosion resistance but also taking all measures to reduce aggressiveness of the coolant medium, water [4, 7, 8]. The primary source of harmful impurities is water from the water treatment plant, which is used to compensate for the loss of water coolant in the power plant cycle. The necessary water for the plant production process is usually taken from rivers and lakes.

This technology requires periodic regeneration [9, 10] of the filters. Regeneration of ion-exchange filters results in highly mineralized, acidic, and alkaline waste water [10]. After circulating through the energy plant, it is a highly mineralized aqueous solution. The high volume of water used produces an increase in the salinity of rivers and lakes when it is returned and causes harmful environmental impact due to the deterioration of the quality of the water. Approximately

25–30% of the water purifier output is for water treatment facility needs. For example, given a thermal power plant with 1200 MW of power, the water treatment plant capacity will be approximately $250\,\text{m}^3$/hour; that is, an average of approximately $62.5\,\text{m}^3$/hour or $547{,}500\,\text{m}^3$/year of water is used for filter recovery. The switching from filtering (water treatment) to backwash, regeneration, and washing modes is carried out either by a time-scheduled mode or based on the volume of passed water and solution. Any of these procedures leads to the consumption of more water and reagents than needed. Thus, it is necessary to find alternative filter operation rules for the aim of reducing the water and reagents consumption. The problem of water treatment for thermal power plants using the ion-exchange method is a multiparametric task. The existing techniques for designing the operation of the water purification plant exclude the possibility of reaching an optimal mode of operation [9, 11, 12].

In this paper we propose a new method based on analysis of the water quality at the filter outlet. That is, we model the dynamics of the ion-exchange process at the filter, and then we solve an inverse problem of finding values for the process parameters. In other words, one can make decisions based on the real work conditions of the equipment. The operation of the water treatment plant under those operating rules can increase the operating cycle of the ion-exchange filter. The amount of waste water and water consumed for its own needs can be reduced. The method is easy to implement for water treatment equipment, either in an existing TPP or at the stage of designing a water treatment plant's equipment. That allows one to predict the stopping time of the filtration process and the starting time for a regeneration process.

Section 2 of the paper contains a description of the mathematical model of the ion-exchange filtration process. In Section 3, a description of the method to solve the direct problem is provided. Section 4 describes the statement and the main idea of solving the inverse problem. In Section 5, the method for the inverse problem with one unknown parameter is developed. In Section 6, results of the numerical solution of the inverse problem with two unknown parameters of the model are provided. The final section contains a brief summary of the research conducted.

2. Mathematical Modeling of the Ion-Exchange Filtration Process

Several mathematical models have been proposed to describe the dynamics of ion-exchange processes [13–16]. In general, these models consist of three equations: mass balance equation, kinetic equation, and isotherm equation. The ion-exchange kinetics equation determines the speed of delivery of ions to the surface of the ion-exchanger. Since the system comprises a kinetic equation, this system of equations models an ion-exchange filter operating in nonequilibrium conditions. In the following, we describe each of them as presented in [11].

2.1. Mass Balance Equation. Sorption of an ions mixture by an ion-exchange material is subject to the law of mass conservation. Thus, the mathematical model for the ion-exchange in the filter also includes a mass balance equation:

$$w_{\text{ap}}\frac{\partial C}{\partial x} + \varepsilon\frac{\partial C}{\partial t} + \frac{\partial q}{\partial t} = 0, \quad x \in (0, L),\ t > 0, \qquad (1)$$

where

  (i) w_{ap} is the flow velocity in the free section of the filter in m/sec;

 (ii) ε is the porosity of the ion-exchange material in m^3/m^3;

(iii) $\partial C/\partial x$ is the rate of change of the ion concentration in the solution, $C(x, t)$, along the filter axis (x) in (mEq/kg)/m;

(iv) $\partial C/\partial t$ is the rate of change of the ion concentration in the solution, $C(x, t)$, with respect to time (t) in (mEq/kg)/sec;

 (v) $\partial q/\partial t$ is the rate of change of the ion concentration in the ion-exchange material, $q(x, t)$, at the point x with respect to time (t) in (mEq/kg)/sec;

(vi) L is the thickness of the filter material in m.

2.2. Kinetic Equation. Processes of the anion exchange and cation exchange of fresh natural waters, as well as processes of ion-exchange of condensed water, run in accordance with the mechanism of the external diffusion kinetics. One of the equations that is customarily used to describe the rate of ion-exchange in the external diffusion kinetics is the Nernst kinetics equation [9]. However, the Nernst theory is not always convenient for describing the diffusion kinetics because of the large number of experimental variables in the equation. To overcome this difficulty, a simpler alternative is proposed in [9]. An equation from the general theory of mass transfer is used, which expresses the hypothesis that the rate of ion-exchange is proportional to the deviation of the ion concentration in the sorbent from the corresponding equilibrium value. The equation is mathematically written in the following form:

$$\frac{dq}{dt} = \eta\left(C - \overline{C}\right), \qquad (2)$$

where

  (i) η is the mass transfer coefficient (proportionality) in m^3/m^3;

 (ii) q is the concentration of exchanging ions in the sorbent in mEq/kg;

(iii) C is the concentration of the exchanging ions in the solution in mEq/kg;

(iv) $\overline{C}$ is the equilibrium ion concentration with respect to the value q in the solution in mEq/kg, which borders with the surface of the ion-exchange material, in the filtration case $C > \overline{C}$.

2.3. Exchange Isotherm Equation. The adsorption isotherm equation is used to determine the capacity of each sorbent for various sorbates. In the ion-exchange theory, isotherms of Langmuir [17], Freundlich [18], and Redlich-Peterson [19] are commonly used. These studies have shown that, for a mathematical description of the ion-exchange process in nonequilibrium conditions, the Langmuir isotherm equation described in [9] may be used. The corresponding mathematical expression can be written as follows:

$$\overline{\varphi} = \frac{(1 - \varphi_a)\,\theta}{k + (1 - k)\,\theta}. \tag{3}$$

Here, we get that

(i) $\overline{\varphi} = \overline{C}/C_0$ is the relative concentration of exchanging ions in the solution phase in mEq/kg, where C_0 is the maximal possible concentration of exchanging ions in the original solution and k is the constant of the exchange isotherm ($k > 1$ for a filtration process and $k < 1$ in a regeneration case);

(ii) φ_a is the relative concentration of additional ions in the ion-exchange material. These ions form a weakly dissociated compound. $\varphi_a = C_a/C_0$ where C_a is the concentration of ions in the original solution in mEq/kg that form a weakly dissociated compound;

(iii) θ is the relative concentration of exchanging ions in the ion-exchange phase in mEq/kg. $\theta = q/q_0$, where q_0 is the total exchange capacity of the ion-exchange material.

Thus, taking into account (1)–(3), the mathematical model of the ion-exchange filtration process for nonequilibrium conditions can be written as follows:

$$\varepsilon \frac{\partial C}{\partial t} + w_{\text{ap}} \frac{\partial C}{\partial x} + \frac{\partial q}{\partial t} = 0,$$

$$\frac{\partial q}{\partial t} = \eta \left(C - \overline{C} \right), \tag{4}$$

$$\overline{\varphi} = \frac{(1 - \varphi_a)\,\theta}{k + (1 - k)\,\theta}.$$

Because exchange isotherm equation (3) is expressed in terms of relative concentrations of exchanging ions in the solution phase and the ion-exchange phase, we can write the equation of balance and kinetics in terms of relative concentrations. By dividing the equation of (1) by the value of C_0 and the equation of (2) by the value of q_0, we rewrite (4) in terms of the functions $\varphi(x,t) = C(x,t)/C_0$ and $\theta = q(x,t)/q_0$, given that $\overline{C} = C_0\overline{\varphi}$:

$$\frac{\partial \varphi}{\partial t} + \frac{w_{\text{ap}}}{\varepsilon} \frac{\partial \varphi}{\partial x} + \frac{q_0}{C_0 \varepsilon} \frac{\partial \theta}{\partial t} = 0;$$

$$\frac{d\theta}{dt} = \frac{\eta C_0}{q_0} \left(\varphi - \overline{\varphi} \right); \tag{5}$$

$$\overline{\varphi} = \frac{(1 - \varphi_a)\,\theta}{k + (1 - k)\,\theta}.$$

Let us introduce the following notations for the dimensionless constants appearing in the system of equations:

$$c = \frac{w_{\text{ap}}}{\varepsilon};$$

$$\beta = \frac{q_0}{C_0 \varepsilon};$$

$$\gamma = \frac{\eta C_0}{q_0}; \tag{6}$$

$$m = (1 - \varphi_a).$$

$0 < m < 1$ is a constant dealing with possible chemical reactions with impurities of other ions in solution.

Given the notations in (6), the system of equations in (5) can be rewritten as

$$\frac{\partial \varphi}{\partial t} + c \frac{\partial \varphi}{\partial x} + \beta \frac{\partial \theta}{\partial t} = 0,$$

$$\frac{\partial \theta}{\partial t} = \gamma \left(\varphi - f(\theta) \right),$$

$$t \in (0, T], \quad x \in (0, L), \tag{7}$$

$$\overline{\varphi} = f(\theta) \equiv \frac{m\theta}{k + (1 - k)\,\theta}.$$

Here, we use the function $f(\theta)$ to denote the relationship between the relative concentration of exchanging ions in the solution phase $\overline{\varphi}$ and the relative concentration of exchanging ions in the ion-exchanger phase θ:

$$\overline{\varphi}(\theta) = f(\theta) \equiv \frac{m\theta}{k + (1 - k)\,\theta}. \tag{8}$$

The result is the system of equations in (7) that describes the model of the ion-exchange filter operating under nonequilibrium conditions. The following are boundary conditions for system (7):

$$\varphi(0, t) = \varphi_0(t), \quad 0 \le \varphi_0(t) < 1,$$

$$\varphi(x, 0) = 0, \tag{9}$$

$$\theta(x, 0) = 0.$$

The physical meaning of these terms is as follows. The condition $\varphi(0, t) = \varphi_0(t)$ indicates that, over the ion-exchanger layer ($x = 0$), at any time t, there is a solute with constant concentration $\varphi_0(t)$. $\theta(x, 0) = 0$ shows that initially ($t = 0$) the absorbed ion is absent at any level of layer x of the ion-exchanger. The equation $\varphi(x, 0) = 0$ indicates that, at the initial time ($t = 0$), the concentration of ions absorbed from the solution in the filter material is negligibly small.

Calculations showed that a change in porosity of the ion-exchange material ε virtually had no impact on the period of time before reaching the permissible concentration of the ion to be removed at the output of the filter, so the average value of 0,325 is used for calculation.

3. The Numerical Solution of the Direct Problem

Direct problem (7), (9) with known constants k and m is nonlinear; however, the nonlinear function $f(\theta)$ satisfies the Lipschitz condition, so it can be shown that the solution of problem (7), (9) exists and is unique. The proof of the uniqueness and existence of the solution to the direct problem is out of the scope of this study. For the numerical solution of problem (7), (9) we apply the finite-difference method. According to this method, the partial derivatives in the system of equations of (7), (9) are replaced with their difference analogues:

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\tau} + c\frac{\varphi_i^{n+1} - \varphi_{i-1}^{n+1}}{h} + \beta\gamma\left(\varphi_i^n - f\left(\theta_i^n\right)\right) = 0,$$

$$\frac{\theta_i^{n+1} - \theta_i^n}{\tau} = \gamma\left(\varphi_i^n - f\left(\theta_i^n\right)\right), \quad t \in (0, T], \; x \in (0, L), \quad (10)$$

$$f\left(\theta_i^n\right) = \frac{m\theta_i^n}{\left(k + (1-k)\,\theta_i^n\right)},$$

$$\varphi_i^0 = 0,$$

$$\theta_i^0 = 0,$$

$$i = 1, 2, \ldots, N, \quad (11)$$

$$\varphi_0^n = \varphi_0 = \text{const}, \quad n = 0, 1, \ldots, N_T.$$

Here, $\tau = T/N_T$ is the time step, and $h = L/N$ is the step in space on a uniform grid.

The first equation of the direct problem is approximated by the implicit difference scheme of point-to-point computation, since when using the calculation parameters characteristic of the technological process the explicit scheme appeared to require a very small step equal to, in terms of time, $\tau = 0,000014$ for $N = 128$. Due to the nonlinear nature of the problem, in order to ensure consistency of the calculation, the time step to be used for the point-to-point computation must be equal to $\tau = 0,000125$ for $N = 128$. The deviation in the results of calculations using the explicit scheme and the point-to-point computation scheme was calculated using the following formula:

$$\delta \triangleq \max_j \frac{\left|\varphi_1^{\text{im}}\left(t_j\right) - \varphi_1^{\text{ex}}\left(t_j\right)\right|}{\text{avg}\left|\varphi_1^{\text{im}}\left(t_j\right)\right|}, \quad (12)$$

where $\varphi_1^{\text{im}}(t_j)$ is the relative concentration of Na^+ cation to be removed at the outlet of the filter when calculating using the implicit finite-difference scheme; $\varphi_1^{\text{ex}}(t_j)$ is the relative concentration of Na^+ cation to be removed at the outlet of the filter when calculating using the explicit finite-difference scheme.

The deviation was equal to 0,075%. To investigate the influence of parameters k and m on the output data the grids of parameters k and m are given at their characteristic ranges of variation. Then, for each pair of discrete values of k and m,
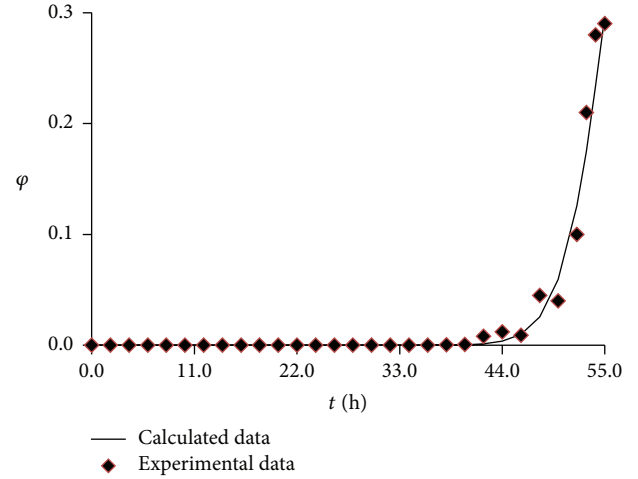

FIGURE 1: The dependence of φ on t.

the concentration function $\varphi_1(t)$ is calculated at the output of the filter on a grid of time values.

We compared the results with data from a real case. The data were collected at the 1200 MW thermal power plant located in the Pavlodar Region of the Republic of Kazakhstan. At the thermal power plant, a 3-stage scheme of deep water desalination is provided, and the capacity of the main water treatment plant is 300 t/h.

Calculations are made for the values $w_{\text{ap}} = 5.55 \times 10^{-3}$ m/sec, $\varepsilon = 0.325$ m^3/m^3, $\beta = 2.5 \times 10^3$, $L = 2.5$ m, and $C_0/q_0 = 2.5 \times 10^{-3}$, which are typical for the hydrogen-cation exchange filters used at thermal power plants in the first stage of water treatment.

In Figure 1, we show the characteristic graph of φ depending on t at filter layer $x = 2,5$ m.

Figure 1 shows changes in the relative concentration of Na^+ cations in time during operation of the filter in the water filtration mode at the output of the filter according to experimental and calculation data. According to the calculations, the relative concentration of Na^+ cations during the first 40 hours of the filter operation is extremely low, ranging from 0.000178 to 0.000477; then breakthrough of Na^+ cations is observed which leads to an increase in the relative concentration of Na^+ cations at the output from the filter. The filtering process ends when the maximum of the relative concentration of Na^+ cations at the output of the filter is achieved equal to 0.297, with the filtration duration being 55 hours. According to the experiment data, the maximum relative concentration of cation removed is achieved at the moment in time being 55 hours. Comparison of the graphs shows that the mathematical model approximation (7), (9) using implicit finite-difference scheme (10) provides satisfactory results.

In Figure 2, we show the characteristic graph of φ depending on x.

Figure 2 shows changes in the relative concentration of Na^+ cations depending on the height of the layer of the ion-exchange material in the filter based on calculation data 20 hours after the beginning of the filtration process. When
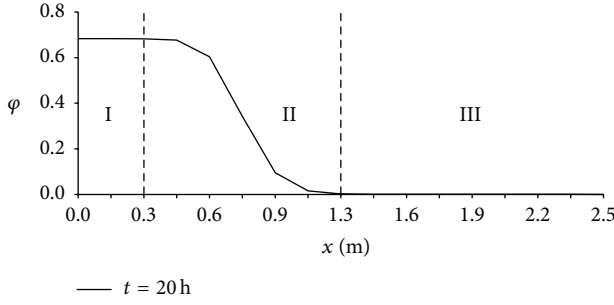
FIGURE 2: The dependence of φ on x.

filtering water through the ion-exchanger layer, the ion-exchange process flows layer by layer. The total height of the ion-exchange layer is 2.5 m. The graph shows three zones as follows: 0 to 0.3 m high layers of depleted ion-exchanger, which cease to be part of the ion-exchange processes (I); 0.3 to 1.3 m high working ion-exchanger layers in which the ion-exchange processes take place (II); and 1.3 to 2.5 m high layers of fresh ion-exchanger which are not yet involved in the ion-exchange processes (III). As the depletion progresses the upper layers of the ion-exchanger cease to be part of the ion-exchange processes. Instead of them fresh ion-exchanger layers are involved in operation which lie under the working layer, and the ion-exchange zone progressively moves as the water treatment process continues.

4. Formulation of the Inverse Problem

During the operation process, the measurement of the impurities concentration at the outlet of the filter is available:

$$\varphi(L, t) = \varphi_1(t), \quad 0 < t < T. \tag{13}$$

Here, T is the horizon observation time.

Due to the complexity of the sorption process and heterogeneity of the mixture to the filter, the parameters γ in model (7) and k and m in (8) cannot be determined accurately. In practice, we can operate with approximate values of k, m, and γ. In some cases, when the main ions of the filtered mixture are known, we can assume that the value of k is given. Then, we still have two uncertain model parameters, the exchange isotherm parameter m and parameter γ. Having the measurements of (13), the problem is actually reduced to an inverse problem, which can be stated as follows:

Find the model parameters m and γ of problem (7), (9) via boundary measurements (13).

Although there are examples of formulations and solutions of inverse problems for filtration processes in the literature [20], this statement of the inverse problem is new. The standard method to solve inverse problems is quasisolution [21], according to which the unknown parameters of the model are determined by minimizing the residual function.

Earlier, in [22], we investigated the behavior of the residual function of the following form:

$$J(k, m) = \frac{1}{2} \int_0^T \left(\varphi(L, t; k, m) - \varphi(L, t; k_0, m_0) \right)^2 dt \tag{14}$$

with the fixed value of the mass transfer coefficient γ. On the basis of the direct numerical simulation described in [23], we have shown that function (14) is not convex. Additionally, the low sensitivity of function (14) with respect to the model parameters k and m is established. This means that the routine use of gradient methods is inefficient. As a result, we propose an alternative approach to the solution of the formulated inverse problem. The main idea of the method is the following; as we have two unknown parameters of the model, m and γ, it is necessary to find at least two integral characteristics of measured data (13), which clearly define these parameters.

5. Solution of the Inverse Problem with One Unknown Parameter, m, of the Model

For solving the inverse problem of finding two unknown parameters m and γ first consider the solution for a simple problem. We solve the problem with one unknown parameter m of the model. Assume first that the parameters k and γ in model (7), (9) are known and state the problem of determining the value of m. The natural measured value is the total amount of impurity Q passed through during the ion observation period:

$$Q(k, m, \gamma) = \int_0^T \varphi_1(t) \, dt. \tag{15}$$

Due to the extremely large scatter of $Q(k, \gamma, m)$, it is more convenient to use its logarithm, $I_1 = \log Q$. It is established numerically that the function $\varphi_1(t)$ and the value I_1 depend on the ratio $s = k/m$. This fact indicates that, using measured data (13), it is possible to recover the ratio $s = k/m$, and it might be difficult to recover the variables k and m simultaneously. It follows that the models with the same value of the function $s(k, m) = k/m$ are equivalent with respect to measured data (13) and observed value of $I_1 = \log Q$. In Figures 3 and 4, we show the characteristic graphs of $\log Q$ depending on s and m.

Thus, the following equivalence principle is obtained for the problem of filtration (7)–(9): *mathematical models with different m and k and the same s = k/m are equivalent with respect to the observed value I_1 and measured data* (13).

This result seems to be natural if we expand the function $f(\theta)$ with respect to θ as follows:

$$f(\theta) = \frac{m\theta}{k + (1 - k)\theta} = \frac{m}{k}\theta + \frac{m(k-1)}{k^2}\theta^2 + \cdots. \tag{16}$$

One can see that the function $f(\theta)$ can be approximated as $f(\theta) = \theta/s$ and depends on the ratio $s = k/m$ for small values of θ. Note that work parameters of the filter use small values of θ, which explains why we obtain the same output data with the same value of the ratio s for different k and m.

TABLE 1: The exact (s_{exact}) and restored (s_{rest}) parameter s values.

Parameters	Parameter values								
s_{exact}	1.45	1.7	2.0	2.45	3.1	3.5	4.0	4.45	4.7
s_{rest}	1.453	1.71	2.14	2.453	3.12	3.52	4.14	4.451	4.71
$\widetilde{\delta}_s$	0.2	0.58	7	0.12	0.65	0.57	3.5	0.02	0.21

$\widetilde{\delta}_s$: relative calculation error s, %.
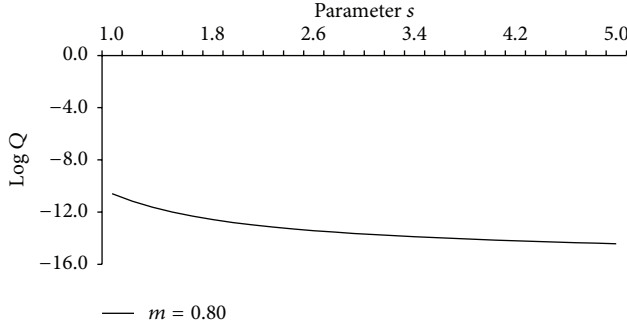
FIGURE 3: The dependence of $\log Q$ on the parameter s.
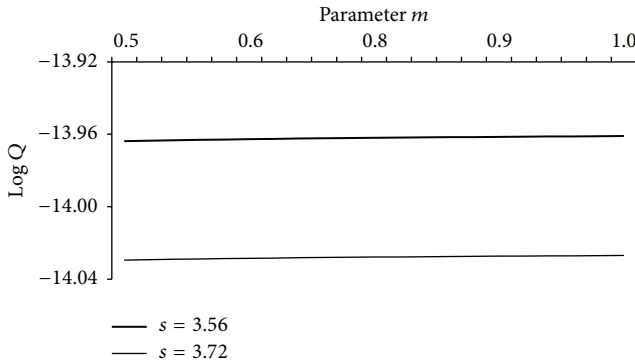
FIGURE 4: The dependence of $\log Q$ on the parameter m.

Calculations show monotonic dependence $I_1(s)$ of s in the practically acceptable range of k and m. This implies that if we know the value of k, then, on the basis of the observed value of I_1, the value of $s = k/m$ is uniquely determined, and, through it, in turn, the value of $m = k/s$ can be calculated. Thus, we have two uncertain parameters of the model, the parameters γ and $s = k/m$, which is associated with exchange isotherm (3). For practical applications of this result, we have generated a table of values of $I_1 = \log Q$ for a range of values of s in the interval $[1.0, 5.0]$. It is enough to interpolate the data of the generated table to recover the desired value of s_0 using the measured value of $\log Q_0$. Table 1 shows the values of the exact (s_{exact}) and restored (s_{rest}) parameter s values for hydrogen-cation exchange filters used in the first stage of make-up water treatment.

The test results showed satisfactory accuracy of s variable restoration.

6. Restoring Parameters m and γ

Suppose now that we know parameter k and do not know two parameters, m and γ. To calculate the range of change of γ, we can use definition (6) of γ:

$$\gamma = \eta \cdot \frac{C_0}{q_0}. \tag{17}$$

In practice, parameter η is calculated according to [9, 24] using the empirical formula

$$\eta \approx \frac{0.009 \alpha w_{\text{ap}}^{0.53}}{d^{1.47}}, \tag{18}$$

where w_{ap} is the rate of flow of fluid in the unit in m/s, d is the ion-exchange grain size in m, and α is an empirical coefficient.

For the calculation, we use the parameter values that are typical for the hydrogen-cation exchange unit of the first stage of water treatment, $w_{\text{ap}} = 0{,}0056$ m/s, and the value of d for the ion-exchange material varies from 0.315 to 1.250 mm. The coefficient α for the exchange of H^+ ions for Na^+ is 1. Based on this data, the values of γ in the processes of interest are in the range of $1.523 \times 10^3 \leq \gamma \leq 3.165 \times 10^3$. Suppose that another observable quantity that is sensitive to the values of the unknown parameters of the model is the logarithm of the impurities concentration at the outlet of the filter at time $t = T$:

$$I_2(k, m, \gamma) = \log(\varphi_1(T)). \tag{19}$$

By solving the direct problem in the range of variation of parameters s and γ, we have generated tables of values of data for $I_1(s, \gamma)$ and $I_2(s, \gamma)$. Based on these two tables, we can calculate the appropriate values of s_0 and γ_0 from the measured values of $I_{1,0}$ and $I_{2,0}$. Below is described a numerical method for calculating s_0 and γ_0. Thus, suppose that we have a table of values for the two measured variables at the filter outlet, $I_1(s_i, \gamma_j)$ and $I_2(s_i, \gamma_j)$. Suppose that $I_{1,0}$ and $I_{2,0}$ are measured values. Using the tables, we can determine a pair of values, s_k, γ_l, for which the minimum deviation is reached:

$$\left\| I_1(s_k, \gamma_l) - I_{1,0} \right\|^2 + \left\| I_2(s_k, \gamma_l) - I_{2,0} \right\|^2$$
$$= \min_{i,j} \left\| I_1(s_i, \gamma_j) - I_{1,0} \right\|^2 + \left\| I_2(s_i, \gamma_j) - I_{2,0} \right\|^2. \tag{20}$$

TABLE 2: The values of the exact and recovered parameters γ and m.

Parameters	Parameter values							
$\gamma_{\text{exact}} \times 10^3$	1.6	1.8	2.0	2.2	2.4	2.6	2.8	3.0
s_{exact}	1.6	2.0	2.4	2.8	3.2	3.6	4.0	4.4
$\gamma_{\text{rest}} \times 10^3$	1.599	1.795	2.002	2.208	2.396	2.588	2.787	2.999
s_{rest}	1.6	1.99	2.4	2.79	3.2	3.59	3.9	4.4
$\widetilde{\delta_\gamma}$	0.06	0.28	0.1	0.36	0.17	0.46	0.46	0.03
$\widetilde{\delta_s}$	0	0.5	0	0.36	0	0.28	2.5	0

$\widetilde{\delta_\gamma}$: relative calculation error γ, %; $\widetilde{\delta_s}$: relative calculation error s, %.

TABLE 3: The values of the mean relative errors δs and $\delta \gamma$ depending on different measurement errors ε.

$S\_$exact	$\gamma\_$exact, 10^{-3}	$\varepsilon = 1\%$		$\varepsilon = 3\%$		$\varepsilon = 5\%$		$\varepsilon = 7\%$	
		δs (%)	$\delta\gamma$ (%)	δs (%)	$\delta\gamma$ (%)	δs (%)	$\delta\gamma$ (%)	δs (%)	$\delta\gamma$ (%)
1.6	1.6	0.0	0.6	0.0	0.8	0.0	1.9	0.0	2.3
1.6	2.0	0.0	0.8	0.0	1.6	0.2	2.9	0.0	3.2
2.0	1.6	0.5	2.1	1.0	3.1	1.0	3.1	2.8	3.6
2.0	2.0	0.3	1.8	1.0	1.9	2.3	13.5	2.8	13.5
2.6	2.0	0.4	14.6	1.3	14.6	2.2	12.2	3.0	6.7

Assuming that the quantities $I_1(s, \gamma)$ and $I_2(s, \gamma)$ are smooth functions of their arguments, we can write approximate equations at a point of s_k, γ_l:

$$
\begin{aligned}
I_{1,0} &= I_1\left(s_0, \gamma_0\right) \\
&= I_1\left(s_k, \gamma_l\right) + \frac{\partial I_1}{\partial s}\left(s_k, \gamma_l\right)\left(s_0 - s_k\right) \\
&\quad + \frac{\partial I_1}{\partial \gamma}\left(s_k, \gamma_l\right)\left(\gamma_0 - \gamma_l\right), \\
I_{2,0} &= I_2\left(s_0, \gamma_0\right) \\
&= I_2\left(s_k, \gamma_l\right) + \frac{dI_2}{ds}\left(s_k, \gamma_l\right)\left(s_0 - s_k\right) \\
&\quad + \frac{\partial I_2}{\partial \gamma}\left(s_k, \gamma_l\right)\left(\gamma_0 - \gamma_l\right).
\end{aligned}
\tag{21}
$$

The partial derivatives $\partial I_1(s_k, \gamma_l)/\partial s, \partial I_1(s_k, \gamma_l)/\partial \gamma, \partial I_2(s_k, \gamma_l)/\partial s$, and $\partial I_2(s_k, \gamma_l)/\partial \gamma$ are approximately calculated using the tables via formulas of finite differences. The relations in (21) represent a linear system of equations with indeterminate s_0, γ_0. This system is solved numerically and defines approximate values of the unknown parameters. Table 2 shows the values of the exact ($\gamma_{\text{exact}}, s_{\text{exact}}$) and restored ($\gamma_{\text{rest}}, s_{\text{rest}}$) parameters γ and s for the hydrogen-cation exchange filters used in the first stage of make-up water treatment.

The test results show satisfactory accuracy of m and γ variable recovery.

The developed method of recovering the parameters was verified with errors ±1%, ±3%, ±5%, and ±7% entered in the exact values Q, $\varphi_1(T)$. The mean relative errors of s and γ parameters recovery are shown in Table 3.

7. Conclusion and Discussions

In the paper a mathematical model of the ion-exchange filter operation mode is considered (7), (9). The direct problem for the ion-exchange filter model was numerically solved. For calculation it is necessary to know the values of m and γ, which in practice are not available for measurement. In the paper a method for the determination of these coefficients based on the output values of ion absorbed at the outlet of the filter was proposed; the inverse problem was formulated. The method is based on the definition of the integral characteristics of the input data that accurately describe these parameters. The integral characteristics were determined. The integral characteristics are the logarithm of the number of impurity ions passing through during the observation period and the increase of the logarithm of the concentration of impurities at the outlet of the filter. The inverse problem was numerically solved given the unknown m and γ parameters. Resetting the parameters using the proposed method yielded satisfactory results.

The developed method can be used in simulation of the ion-exchange unit operation mode. This will allow determining the optimal mode of operation facilitating reduction of the amount of regeneration and washout water.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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References

[1] H. J. Fortune, "Boiler feed-water treatment for corrosion control—part 2," *Anti-Corrosion Methods and Materials*, vol. 9, no. 6, pp. 154–156, 1962.

[2] N. A. Mesherskiy, *Operation of Water Treatment Plants Power of High Pressure*, Energoatomizdat, Moscow, Russia, 1984 (Russian).

[3] L. N. Sidelkovsky and V. N. Yurenev, *Boilers Industrial Enterprises: A Textbook for High Schools*, Energoatomizdat, 3rd edition, 1988, (Russian).

[4] S. A. Avlonitis, M. Pappas, K. Moutesidis, D. Avlonitis, K. Kouroumbas, and N. Vlachakis, "PC based SCADA system and additional safety measures for small desalination plants," *Desalination*, vol. 165, pp. 165–176, 2004.

[5] M. R. Choudhury, M.-K. Hsieh, R. D. Vidic, and D. A. Dzombak, "Corrosion management in power plant cooling systems using tertiary-treated municipal wastewater as makeup water," *Corrosion Science*, vol. 61, pp. 231–241, 2012.

[6] A. Phongphiphat, C. Ryu, Y. B. Yang et al., "Investigation into high-temperature corrosion in a large-scale municipal waste-to-energy plant," *Corrosion Science*, vol. 52, no. 12, pp. 3861–3874, 2010.

[7] V. Slobodan, V. Nikola, and D. Željko, "Power electronics solution to dust emissions from thermal power plants," *Serbian Journal of Electrical Engineering*, vol. 7, no. 2, pp. 231–252, 2010.

[8] V. A. Prisyazhniuk, "Alternative trends in development of thermal power plants," *Applied Thermal Engineering*, vol. 28, no. 2-3, pp. 190–194, 2008.

[9] A. A. Gromoglasov, A. C. Kopylov, and A. V. Pil'shikov, *Water Treatment Processes and Machines*, Energoatomizdat, 1990, (Russian).

[10] A. I. Glazyrin, L. P. Muzyka, and M. M. Kabdualieva, *Preparation of Water for Thermal Power Plants and Industrial Enterprises/Tutorial/*, Republican Publishing Office, Almaty, Kazakhstan, 1997 (Russian).

[11] Y. M. Kostrikin, N. A. Mishersky, and O. V. Korovin, *Water Treatment and Water Regime of Power Low and Medium Pressure, Handbook*, Energoatomizdat, Moscow, Russia, 1990 (Russian).

[12] O. V. Livshic, *Handbook of Water Treatment of Boiler Plants*, Energy, Moscow, Russia, 1976 (Russian).

[13] V. L. Bogatyryov, "Clathrate-forming ion exchangers," *Solvent Extraction and Ion Exchange*, vol. 16, no. 1, pp. 223–265, 1998.

[14] T. Bolanča and Š. Cerjan-Stefanović, "Optimization strategies in ion chromatography," *Journal of Liquid Chromatography & Related Technologies*, vol. 30, no. 5–7, pp. 791–806, 2007.

[15] J. A. Davis and D. B. Kent, "Surface complexation modeling in aqueous geochemistry," *Reviews in Mineralogy and Geochemistry*, vol. 23, no. 1, pp. 177–260, 1990.

[16] Z. Wang and D. E. Giammar, "Mass action expressions for bidentate adsorption in surface complexation modeling: theory and practice," *Environmental Science and Technology*, vol. 47, no. 9, pp. 3982–3996, 2013.

[17] I. Langmuir, "The constitution and fundamental properties of solid and liquids—part 1 solids," *Journal of the American Chemical Society*, vol. 40, pp. 1361–1403, 1918.

[18] H. Freundlich, "Uber die adsorption in Losungen," *Zeitschrift für Physikalische Chemie*, vol. 57, pp. 385–471, 1906.

[19] L. Jossens, J. M. Prausnitz, W. Fritz, E. U. Schlünder, and A. L. Myers, "Thermodynamics of multi-solute adsorption from dilute aqueous solutions," *Chemical Engineering Science*, vol. 33, no. 8, pp. 1097–1106, 1978.

[20] M. G. Tokmachev, *Mathematical modeling of reagent-free multicomponent cyclic ion-exchange process of desalination of natural waters [Dissertation on Competition of a Scientific Degree of the Candidate of Physical and Mathematical Sciences]*, 2008, (Russian).

[21] A. Tikhonov and V. Arsenin, *Solutions of Ill-Posed Problems*, John Wiley & Sons, New York, NY, USA, 1977.

[22] B. G. Mukanova and N. S. Glazyrina, "Numerical modeling of the ion-exchange filter work," *Herald of the ENU, Series of Natural and Technical Sciences, Astana*, no. 1, pp. 20–26, 2014 (Russian).

[23] E. Kamke, *Differentialgleichungen. Lösungsmethoden und Lösungen II. Partielle Differentialgleichungen 1. Ordnung für eine Gesuchte Funktion*, Leipzig, 1944.

[24] Y. M. Zagray, A. M. Koganovsky, and L. A. Kulskiy, *Ion-Exchange Purification of Industrial Waste Water in a Fluidized Bed Cation Exchangers*, Publishing Ukr NIITI, Kiev, Ukraine, 1966 (Russian).