

Multiparametric Optimization of Water Treatment Process for Thermal Power Plants

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Abstract—The formulated problem of optimization of the technological process of water treatment for thermal power plants is considered in this article. The problem is of multiparametric nature. To optimize the process, namely, reduce the amount of waste water, a new technology was developed to reuse such water. A mathematical model of the technology of wastewater reuse was developed. Optimization parameters were determined. The model consists of a material balance equation, an equation describing the kinetics of ion exchange for the non-equilibrium 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. A direct problem of calculating the impurity concentration at the outlet of the water treatment plant was numerically solved. The direct problem was approximated by an implicit point-to-point computation difference scheme. The inverse problem was formulated as relates to determination of the parameters of the mathematical model of the water treatment plant operating in non-equilibrium conditions. The formulated inverse problem was solved. Following the results of calculation the time of start of the filter regeneration process was determined, as well as the period of regeneration process and the amount of regeneration and wash water. Multi-parameter optimization of water treatment process for thermal power plants allowed decreasing the amount of wastewater by 15%.

Keywords—Direct problem, multiparametric optimization, optimization parameters, water treatment.

I. INTRODUCTION

OPERATION of the equipment of modern power plants is characterized by high thermal loads, which requires the provision of high quality water-coolants in order to prevent the formation of scale and a sharp decline in the efficiency of the energy source [1]. Corrosion processes are intensified under the resulting scale which leads to destruction of the metal of working heating surfaces [2]-[6]. The primary source of harmful impurities is make-up water from the water treatment plant used to compensate for loss of water coolant in the power plant cycle.

The most stringent requirements for the make-up water quality are established at packaged thermal power plants where boilers are operated under supercritical pressure [7]. The research work was carried out using the existing

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equipment of the 300 MW thermal power plant and Пn-950-255 straight-through boilers with intermediary reheat of steam, steam-generating capacity being 950 t/h of superheated steam at a pressure of 255 kgf/cm² and temperature of 565°C. At the thermal power plant make-up water treatment is carried out at the water treatment plant in two stages:

1. pre-treatment of water (raw water heating, water clarification in water clarifiers mechanical filters)
2. deep water purification by ion exchange (the technology of three-stage sequential H-OH-ionizing).

Three-stage H-OH-ionizing pattern consists of consecutively arranged cationite and anion-exchanging filters through which water is passed for deep cleaning.

Ion-exchange filters operation includes four stages: filtration, ion-exchange material backwash, regeneration of ion-exchange material and ion-exchange material washing-off [8]. During filtration, when ion exchanger transforms from one ionic form to another, a reduction in its particles' diameter takes place due to the uneven spatial distribution of divinylbenzene and the functional groups in ion exchanger grains. This enables the most compressible grains to move, and the loosest layers of the ion exchanger to condense [8]. The resulting reduction in the porosity of the ion exchanger layer during the process causes its hydraulic resistance to increase. Therefore, the filtration step is followed by backwashing of the filter layer which results in a rearrangement of the ion exchanger from a denser to a looser layer with simultaneous removal of particles. During backwash the ion exchange grains are entrained by upward flow of water and, after some distance, fall down. Thus, ion exchanger grains of various ionic forms are more or less evenly distributed over the height of the loosened layer of the ion exchanger.

In order to restore the exchanging ability of spent ion exchanger regeneration process is performed. Regeneration is performed by way of passing a regeneration solution through the layer of spent ion exchanger. Regeneration of ion-exchange filters results in highly mineralized, acidic or alkaline waste water. With the continuous circulation of water through the production cycle, when water is taken from the surface sources for the needs of production and is returned as a high-mineralized aqueous solution, in rivers and lakes an increase in salinity can be observed, and consequently, deterioration of water quality, which is a very negative impact on the environment.

Regeneration process is followed by spend ion exchangers wash-off. During the wash-off procedure the regeneration

process products as well as regenerants are removed from the ion exchanger.

About 25-30% of the water purifier output is consumed for own needs of water treatment plants (for processes of backwash, regeneration and washing of ion-exchange material) [8].

These considerations raise relevance of the issue of water treatment plants operation mode optimization which would allow obtaining the desired quality of water used for power plants, reducing the amount of pollution of surface water bodies, and reducing the amount of water for its own needs.

II. THE MINIMUM WASTEWATER AMOUNT DETERMINATION PROBLEM

The problem of determining the minimum amount of wastewater during the water treatment process at thermal power plants is a multiparameter task [9].

The volume of water used for the water treatment plant's own needs is calculated using

$$V = V_{\text{mix}} + V_{\text{reg}} + V_w \quad (1)$$

Here V_w is the amount of water needed to wash-off ion-exchange material, m^3 , V_{reg} is the volume of regeneration solution, m^3 , V_{mix} is the volume of water required for backwashing of ion-exchange material loaded in the water treatment plant, m^3 .

The volume of water for backwashing depends on the area of the filter loaded with the ion exchanger and is calculated as, m^3/reg

$$V_b = fti60/1000, \quad (2)$$

where f is ion-exchange filter area, i is the specific consumption of water for backwashing of ion-exchange material, $\text{dm}^3/(\text{s}\times\text{m}^2)$, t is the period of time for backwashing of ion-exchange material, min .

The volume of backwash water for each filter is a constant value, so this value is ignored when minimizing the amount of water for the water treatment plant's own needs.

The volume of regeneration solution is a function of the relative concentration of displacing ions in the filtrate and is calculated using

$$V_{\text{reg}} = V_0 * \left(\varepsilon + \frac{k}{h(k+(1-k)\varphi)^2} \right) \quad (3)$$

The regeneration solution concentration, the ion exchange constant and full operating capacity are considered to be invariable.

The wash-off process is controlled using the regeneration solution concentration data, i.e. the electrolyte in the wash-off water leaving the filter. The volume of the solution fed for washing is calculated in two stages:

The total consumption of wash-off water for H-cation filter is determined using

$$V_{wk} = 2,607V_0 + 9,36Q + 21,097Q \ln \frac{0,000135}{C_{H^+}} \quad (4)$$

Here V_0 is the amount of cation exchanger loaded in the filter, m^3 , C_{H^+} is the concentration of H^+ ion in the filtrate, mgEq/mL , Q is the flow rate of wash-off water, m^3/min .

The total flow rate of wash-off water for the filter is determined using

$$V_{wa} = 2,485V_0 + 15,8Q + 21,097Q \ln \frac{0,000135}{C_{OH}} \quad (5)$$

Here V_0 is the volume of the anion exchanger loaded in the filter, m^3 , C_{OH} is the concentration of OH^- anion in the filtrate, mgEq/mL , Q is the flow rate of wash-off water, m^3/min [9].

The problem of determining the minimum amount of wastewater can be formulated as:

Determine the minimum volume of wastewater of the water treatment plant.

To solve this problem it is necessary to calculate the coefficient of consumption of water for own needs of all filters of the water treatment plant

$$F = \frac{V_{\text{reg}} + V_w}{V_f} \quad (6)$$

where V_f is the volume of purified water, m^3 .

To determine the minimum of function (6), we considered a mathematical model of the ion exchange process in ion-exchange filter.

III. MATHEMATICAL MODELING OF THE ION-EXCHANGE FILTRATION PROCESS

Many research works have focused on the dynamics of ion exchange for subsequent modeling and calculation of various ion exchange processes [9]-[13]. In general, these models consist of three equations:

- Mass balance equation;
- Kinetic equation;
- Isotherm equation.

The system of differential equations describing the operation of ion-exchange filter operating in non-equilibrium conditions is as

$$\begin{cases} \varphi_t + c\varphi_x + \gamma\beta(\varphi - f(\theta)) = 0, \\ \theta_t = \beta(\varphi - f(\theta)), t \in (0, T], x \in (0, L) \\ f(\theta) = m\theta/(k + (1-k)\theta) \end{cases} \quad (7)$$

with initial-boundary conditions

$$\begin{cases} \varphi(x, 0) = 0, \theta(x, 0) = 0, \\ \varphi(0, t) = \varphi_0(t), 0 \leq \varphi_0(t) < 1 \end{cases} \quad (8)$$

Here $\theta(x, t)$, $\varphi(x, t)$ are concentrations of ion absorbed from the solution in the ion-exchange material and the solution respectively, normalized to q_0 , C_0 – the total exchange capacity of the ion-exchange material and the total concentration of exchanging ions in solution, L – thickness of the ion-exchange material layer. The function $f(\theta)$ determines

the value of the equilibrium concentration of exchanging ion in the solution at a given concentration θ of the same ion in the ion-exchange material. The constant $k > 1$ - the so-called exchange isotherm constant, $0 < m < 1$ - the constant determining possible chemical reactions with other impurities in the solution

May w_{ap} be the average rate of flow of fluid through the apparatus, m/h, determined by the water flow, and ε - the porosity of the ion exchanger loaded in the filter, m^3/m^3 .

The parameters of the model are determined using the following formulas $c = w_{ap}/\varepsilon$, $\beta = q_0/(\varepsilon C_0)$, $\gamma = \eta \cdot C_0/q_0$, η - proportionality factor determining the rate of release of ions from the ion-exchange material. This ratio is called intradiffusion mass transfer coefficient and is determined by chemical kinetics of ion exchange, it depends on the area of free surface of the ion-exchange material pellets, on the rate of filtration, exchanging ion valences. Often the variable η is determined by some empirical relationships, for example, according to [9] $\eta \approx 0.009\alpha w_{ap}^{0.53}/d^{1.47}$ where α is an empirical coefficient, d is the diameter of the granules, m. At this stage of the study, we neglect the change in porosity of the material ε .

IV. NUMERICAL SOLUTION OF THE DIRECT PROBLEM

The direct problem (7) with known constants k and m is nonlinear; however, the nonlinear function $f(\theta)$ satisfies the Lipschitz condition [14], so it can be shown that the solution of problem (7)-(8) exists and is unique. For the numerical solution of the direct problem (7)-(8) we used the finite differences method. The direct problem was approximated by an implicit point-to-point computation difference scheme because when calculating the parameters typical for the process, it turned out that the explicit scheme required a very small step. It turned out that due to the nonlinear nature of the problem a little time step is required for calculation stability even for point-to-point computation.

Calculations are made for the values $w_{ap} = 5.55 \times 10^{-3}$ m/sec, $\varepsilon = 0.4$ m^3/m^3 , $\gamma = 2500$, $L = 1.8$ m, and $C_0/q_0 = 5.75 \times 10^{-3}$, which are typical for the hydrogen-cation exchange filters used at thermal power plants in the first stage of water treatment. In Fig. 1, we show the characteristic graph of φ depending on t at filter layer x .

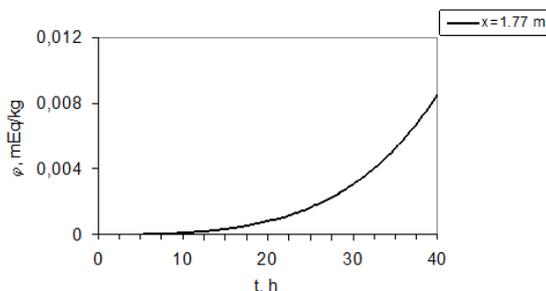


Fig. 1 The dependence of φ on t at the outlet of the filter

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

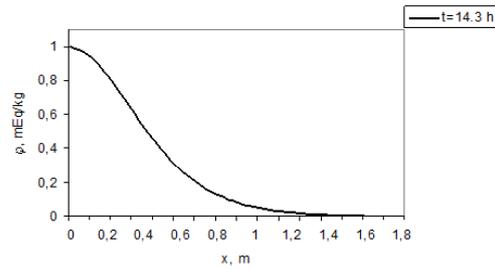


Fig. 2 The dependence of φ on x at the moment $t=14.3$ h

V. FORMULATION OF THE INVERSE PROBLEM

During the monitoring water treatment plants are available for measuring the concentration of impurities at the outlet of the filter

$$\varphi(L, t) = \varphi_1(t), 0 < t < T \quad (9)$$

Here, T is the horizon observation time.

Due to the complexity of the sorption process and heterogeneity of the mixture for filtering, parameter γ in (7), and, k and m in

$$f(\theta; k, m = \frac{m\theta}{k+(1-k)\theta}) \quad (10)$$

cannot be determined accurately and we can only consider just a few effective values of k , m and γ .

Given the fact that we have available measurements (9), the problem is actually reduced to the inverse problem which can be stated as follows:

Find the model parameters m , γ following the results of solutions of (7) on the basis of additional information (8) and calculate the time T^ , at which a maximum permitted output pollutant φ^* concentration is reached.*

If we assume k constant to be known we still have two uncertain model parameters - exchange isotherm parameter m , and parameter γ related to the constant of internal diffusion exchange under formula $\gamma = \eta \cdot C_0/q_0$.

Although there are examples of formulations and solutions of inverse problems for filtration processes in [15], this statement of the inverse problem is new.

The standard method to solve inverse problems is quasisolution [16], according to which the unknown parameters of the model are determined by minimizing the residual function.

Earlier, in [17], we investigated the behavior of the residual function of

$$J(k, m) = \frac{1}{2} \int_0^T (\varphi(L, t; k, m) - \varphi(L, t; k_0, m_0))^2 dt \quad (11)$$

with the fixed value of the mass transfer coefficient γ .

On the basis of the direct numerical simulation described in [17], we have shown that (11) is not convex. Additionally, the

low sensitivity of (11) with respect to the model parameters k and m is established. This means that the routine use of gradient methods is inefficient

In this paper, we propose an alternative approach to the solution of the formulated inverse problem, determination of the optimal process parameters.

The idea of the method is as follows: as we have two unknown parameters of the model, m and γ , it is necessary to find at least two integral characteristics of the measured data (3), which clearly define these parameters.

The natural measured value is the total amount of impurity Q passed through during the ions observation period

$$Q(T, k, m, \gamma) = \int_0^T \varphi_1(t) dt \quad (12)$$

We hypothesized that this is one of the values which is sensitive to the model parameters, and examined its dependence on the k , m values. Due to the extremely large scatter of $Q(T)$ it proved to be more convenient to use its logarithm $I_1 = \log Q$.

It was established that the value I_1 is dependent on the ratio $s = k/m$, and practically does not depend on m . This fact indicates that using the values of variable I_1 it is possible to restore the relationship $s = k/m$, and it is impossible to restore the variable m .

Suppose that another observable quantity that is sensitive to the values of the unknown parameters of the model is the increment of the logarithm of the impurities concentration at the outlet of the filter

$$I_2(T, k, m, \gamma) = \log(\varphi_1(T)) - \log(\varphi_1(0)) \quad (13)$$

By solving the direct problem in the range of variation of parameters s and γ we have generated a table of values of variables $I_1(T, s, \gamma)$ and $I_2(T, s, \gamma)$.

Based on these two tables, we can calculate the appropriate values s_0, γ_0 from the measured values $I_{1,0}$ and $I_{2,0}$, i.e., using the tables, we found a couple of values s_k, γ_l , for which the minimum deviation is achieved

$$\begin{aligned} & \|I_1(s_k, \gamma_l) - I_{1,0}\|^2 + \|I_2(s_k, \gamma_l) - I_{2,0}\|^2 = \\ & = \min_{i,j} \|I_1(s_i, \gamma_j) - I_{1,0}\|^2 + \|I_2(s_i, \gamma_j) - I_{2,0}\|^2 \end{aligned} \quad (13)$$

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

$$I_{1,0} = I_1(s_0, \gamma_0) = I_1(s_k, \gamma_l) + \frac{\partial I_1}{\partial s}(s_k, \gamma_l)(s_0 - s_k) + \frac{\partial I_1}{\partial \gamma}(s_k, \gamma_l)(\gamma_0 - \gamma_l),$$

$$I_{2,0} = I_2(s_0, \gamma_0) = I_2(s_k, \gamma_l) + \frac{\partial I_2}{\partial s}(s_k, \gamma_l)(s_0 - s_k) + \frac{\partial I_2}{\partial \gamma}(s_k, \gamma_l)(\gamma_0 - \gamma_l) \quad (14)$$

The partial derivatives $\frac{\partial I_1(s_k, \gamma_l)}{\partial s}$, $\frac{\partial I_1(s_k, \gamma_l)}{\partial \gamma}$, $\frac{\partial I_2(s_k, \gamma_l)}{\partial s}$, and $\frac{\partial I_2(s_k, \gamma_l)}{\partial \gamma}$ are approximately calculated using the tables via formulas of finite differences.

The relations in (14) 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 I shows the values of the exact ($\gamma_{\text{exact}}, m_{\text{exact}}$) and restored ($\gamma_{\text{rest}}, m_{\text{rest}}$) parameters γ and m for the hydrogen-cation exchange filters used in the first stage of make-up water treatment.

TABLE I
THE VALUES OF THE EXACT AND RECOVERED PARAMETERS γ AND m .

Parameters	Parameter values							
γ_{exact}	6.3	7.5	8.6	9.1	10.5	12.4	17.0	23.7
m_{exact}	0.55	0.6	0.66	0.7	0.73	0.78	0.82	0.85
γ_{rest}	6.35	7.53	8.61	9.21	10.54	12.43	17.15	23.72
m_{rest}	0.57	0.64	0.68	0.72	0.74	0.80	0.82	0.86

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

We used the following equation to calculate the timepoint T^* using which it is possible to achieve the maximum allowable concentration rate of the removed ion φ at the outlet

$$T^* = \frac{xq_0}{w_{\text{ap}}C_0} + \frac{\ln \varphi + 1}{\sigma w_{\text{ap}}^{0.5} d^{-1.5} h^{0.5}} \quad (15)$$

Here h is distributive relations, $h = C_0/q_0$, σ is coefficient depending on the removed ion.

VI. NUMERICAL SOLUTION OF THE PROBLEM OF DETERMINING THE MINIMUM AMOUNT OF WASTEWATER AT THE WATER TREATMENT PLANT

To find the minimum of (6), we calculated the time of operation of each ion-exchange filter at the water treatment plant using (15), the volume of regeneration solution using (3) and calculated the volume of wash-off water for the H-cationite and OH-anion-exchanging filters using (4) and (5).

The volume of water ionized per one cycle of operation of each filter was calculated using

$$V_f = w_{\text{ap}} f T^* \quad (16)$$

where $f = \pi D^2/4$ is the filtration area, m^3 ; D is the filter diameter, m^3 , x is the height of loading of the ion exchanger in the filter, m .

In order to determine the minimum of (6), we used Hooke-Jeeves direct search method.

VII. WASTEWATER REUSE TECHNOLOGY

To optimize the operation of the three-stage desalination scheme, particularly relating to the reduction of the amount of wastewater, a new technology was developed to reuse such water. This technology involves the installation of sodium-cation filters before hydrogen-cation filters. Up to 80% of hardness salts are removed at sodium-cation filters which allows reducing the load on hydrogen-cation filters and the number of regeneration cycles, and, thus, reducing the amount of wastewater. The technology also provides for the reuse of water after backwashing the ion exchange material, before

feeding the regeneration solution, and the use of a portion of wash-off water in the course of backwashing of each filter. Regeneration of the ion exchange material is performed by way of step-by-step countercurrent regeneration using stoichiometric coefficients which results in saving the amount of the regeneration solution by 15%, which in turn reduces the amount of wastewater.

We calculated the three-stage desalination scheme based on engineering calculations used at the thermal power plant [18]. The same scheme was calculated using the mathematical calculations described in the article, as well as application of the wastewater reuse technology. The calculation results are shown in Tables II and III.

TABLE II
THE RESULTS OF CALCULATION OF THE THREE-STAGE DESALINATION SCHEME BASED ON ENGINEERING CALCULATIONS

Name of the filter	Number of working filters	Volume of water for 1 backwashing, m ³	Volume of water for 1 regeneration, m ³	Volume of water for 1 washing, m ³	Regeneration amount per day	Total volume of water per year, m ³
Mechanical	7	60,0	-	-	2	306 600,00
H-cationite stage I	6	60,0	79,79	55,0	0,62	264 485,86
OH-anionite stage I	5	70,0	34,3	55,0	0,71	206 412,98
H-cationite stage II	4	70,0	31,02	55,75	1,03	235 750,73
OH-anionite stage II	2	44,0	13,72	82,5	0,13	13 306,88
H-cationite stage III	4	62,0	31,02	55,75	0,1	21 720,42
OH-anionite stage III	3	21,5	13,72	220,0	0,1	27 946,59
Total volume of water used for own needs water treatment plant per year, m ³						1 076 223,46

TABLE III
THE RESULTS OF CALCULATION OF THE THREE-STAGE DESALINATION SCHEME USING THE MATHEMATICAL CALCULATIONS AND APPLICATION OF THE WASTEWATER REUSE TECHNOLOGY

Name of the filter	Number of working filters	Volume of water for 1 backwashing, m ³	Volume of water for 1 regeneration, m ³	Volume of water for 1 washing, m ³	Regeneration amount per day	Total volume of water per year, m ³	Volume of the clarified water is recycled after backwashing, m ³
Mechanical	4	63,6	0	0	2	185712	29 200
Sodium cationite	2	65,5	23,8	122,9	0,8	123924,8	7 008
H-cationite stage I	2	38,2	0	79,5	0,89	76469,69	5 847,3
H-cationite stage II	3	18,1	52,7	64,9	0,95	141161,9	4 161
OH-anionite stage I	3	28,6	0	143,1	1,06	199292,2	10446,3
OH-anionite stage II	3	44	20,6	107,3	0,09	16940,7	394,2
H-cationite stage III	3	19,1	46,5	57,2	0,05	6727,3	219,0
OH-anionite stage III	2	28,6	20,6	107,3	0,04	5026,8	128,5
Total volume of water used for own needs water treatment plant per year, m ³						755339,0	
Volume of the clarified water is recycled after backwashing per year, m ³							57 404,3

VIII. CONCLUSION

The direct problem for the mathematical model of ion-exchange filter is considered and solved. The inverse problem of determining the parameters of the mathematical model of ion-exchange filter is formulated and solved as well as determining the time required to achieve the maximum permitted concentration of the ion being removed. The new wastewater reuse technology is developed. The problem of determining the minimum amount of wastewater for the power plant's WTP is solved.

The implementation of the technology of reuse of water treatment plant wastewater on industrial equipment resulted in the reduction of wastewater amount by 320 884, 46 m³ per year, with an additional annual inflow into the cycle of clarified water in the amount 57 404,3 m³. That is, the thermal power plant not only discharges an annual total of 378 288,76 m³ of wastewater into the environment, but also saves the same amount of water which might have otherwise been consumed from surface sources.

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