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Technological modeling of physicochemical removal of iron from deep groundwater

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ABSTRACT

In view of the significant difficulties arising in controlling the operation of the rapid iron removal filters on the basis of full exhaustion of their clarifying resource at every calculation stage (filter run), it is suggested to realize a simple control algorithm, which assumes an equal duration of filter runs during the entire service life of one filtering material change. Since the efficiency of physicochemical iron removal depends significantly on the specified duration, in order to establish its optimal value in every given case it is necessary to perform a special technical and economic analysis with a detailed consideration of the composition and degree of contamination of natural water. In the working conditions considered above, which are typical for physicochemical iron removal from deep groundwater in Ukraine, such a value was 600 conventional units, which corresponds to 48 h. The cost of the treatment increases significantly even with a small deviation of the filter run duration from the optimal value.

1. Introduction

Water supply to settlements and industrial plants is conducted from surface or ground sources [1]. Surface waters are often contaminated with toxic chemicals, petroleum products, salts of heavy metals, phenols, biogenic substances, etc. [2]. Groundwater are characterized by physical and bacteriological indicators that are quite constant and their quantity is rather high for economic and drinking water supply, with quite diverse chemical indicators, which do not depend on weather conditions in most cases [3] especially for deep horizons.

Iron is often present in high concentrations in groundwater [4–6]. There are a number of consequences associated with the fact. Continuous consumption of water with a high iron content can lead to a development of various health problems [7,8]. Additionally, a high iron content in water is associated with an unpleasant taste, red color of water and stains on laundry and plumbing fixtures [9]. Different methods are developed and used for iron removal from water [10–13]. The use of sorbents (nanomaterials) is perspective for the sewage treatment from heavy metal ions, including iron [14–16].

In general, reagent-free, reagent, cation-exchange, membrane and biochemical methods can be used at iron removal from water for drinking purposes [17]. The first two methods belong to physicochemical methods and involve the introduction of iron oxidizers. When the first method is applied, this oxidizing agent is air oxygen [17]. The task of the methods is to convert soluble forms of iron into

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insoluble forms ($Fe(OH)_3$). Complete oxidation of iron in tanks with subsequent filtration of water through granular medium of different nature (deep-bed iron removal from water) is possible. When air oxygen is introduced, iron oxidation occurs as follows

$$4Fe^{2+} + 8HCO_3^- + O_2 + 2H_2O = 4Fe(OH)_3\downarrow + 8CO_2\uparrow.$$

At contact iron removal, water after aeration and degassing treatment is released directly into the granular medium. A necessary condition for the effective iron removal is the presence of an active film consisting of iron compounds on the surface of the bed grains, which becomes a catalyst for the process. The grains surface has an electric charge, the field strength of which at the boundary of the adsorption layer is characterized by the value of the electrokinetic potential. Sign and magnitude of the potential, which depend on the pH of the filter medium, affect the adsorption activity of the grains surface [17,18] in relation to particles in the liquid phase. There is adsorption of ferrous oxide ions on the surface of "clean" grains of filtering medium at filtration of groundwater at the first stage. After some time, sorption of the oxidized iron takes place, and the electrokinetic potential of the medium grains decreases, the adsorption properties of the specified surface decrease. At the same time, dissolved oxygen is present in water, under the action of which adsorbed iron oxide ions are oxidized and hydrolyzed. Thus, a deposit is formed, which also becomes a catalyst for the process. After the formation of the "film", adsorption of the ferrous iron ions proceeds in parallel on the free surface of the filter media and on the surface of the deposit. The adsorption properties of the packed bed depend on the specific surface area, i.e. the finer are the grains and the larger are their grain shape coefficient, the more ferrous iron will be adsorbed.

To ensure the necessary adsorption properties, the filter medium can be treated with substances having catalytic properties for oxidation and adsorption of ferrous iron. Also, it is possible to use natural materials containing manganese dioxide (pyrolusite, etc.).

In Ukraine, the reagent-free aeration method is most often used for iron removal from deep groundwater, as it is simpler and cheaper [18]. Natural and artificial materials are used as a granular filtering material [17]. The type of the filter medium and characteristics of its grains significantly affect the efficiency of water iron removal, the size of filter plants and their productivity.

One of the economically rational mediums is polystyrene foam, which has a number of technical and economic advantages [17]. Polystyrene foam filters represent a container in which the polystyrene foam medium is kept in a flooded state by a special construction. We propose to apply the scheme shown in Fig. 1 for iron removal from water. The iron removal from water is conducted in the following way. Initial water through the pipeline 1 goes to the aerator 2, where water saturation with air oxygen and partial degassing of gases dissolved in groundwater (hydrogen sulfide, carbon dioxide, etc.) takes place. Further water enters the filtration rate regulator 3. Aerated water through the pipeline 4 is released to the distribution system 5, evenly distributed over the filter area, passes through the polystyrene foam medium 7 and treated water is collected in the above-filter space 9. Treated water is discharged to the consumers through the pipeline 10. The filter is switched to the washing mode by closing the gate valve on the pipeline 1 and opening the valve on the pipeline 11. Clean water from the above-filter space, moving by downward flow, expands and washes the filter

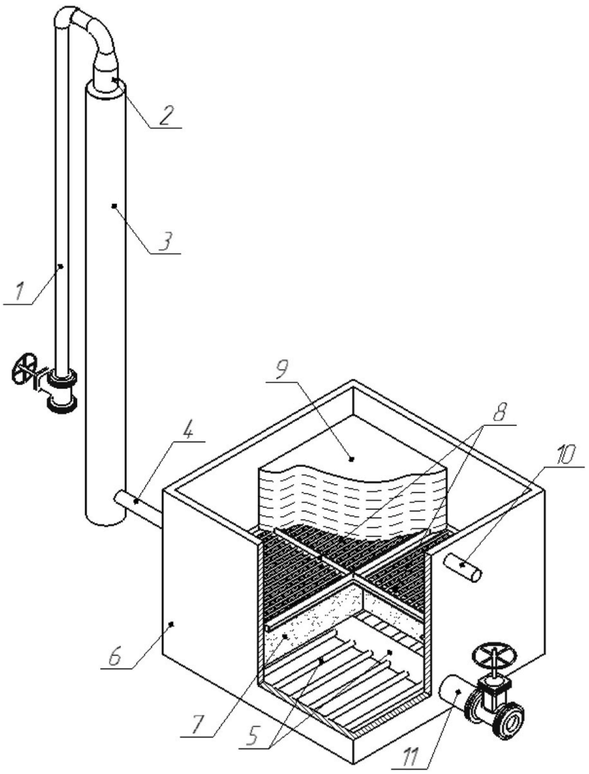

Fig. 1. Scheme of iron removal from water by aeration and filtration on polystyrene foam filters with upflow filtration.

medium. Contaminated washing water is collected by the distribution system 5 and discharged into the sewage system by the pipeline 11. The water level in the above-filter space gradually decreases and when the level reaches 10 cm above the grid, backwashing is stopped by closing the gate valve on the pipeline 11. The filter is again switched to the filtering mode, for which purpose the gate valve on the pipeline 1 is opened.

1 - groundwater supply pipeline; 2 - aerator; 3 - filtration rate regulator; 4 - aerated water pipeline; 5 - bottom distribution system; 6 - filter body; 7 - polystyrene foam medium; 8 - retaining grid; 9 - above-filter (washing) space; 10 - treated water (filtrate) removal pipeline; 11 - washout pipeline.

Various technological schemes and simple calculation methods have been developed to solve the problem of iron removal from deep groundwater [17–19]. However, a number of its important formal peculiarities were not being considered, including nonlinear effects of mass transfer, autocatalyticity of the sorption, specific character of deposit consolidation, etc. Mathematical models adequately describing this technological process have not been proposed until now. This is due to both the complexity of a set the physicochemical processes insuring virtually complete iron removal and the need for specific extensive experimental studies to provide information support for mathematical modelling.

Based on the results of our own experimental data and the conceptual model [18], we have developed a mathematical model of iron removal consisting of interconnected joint clarification and hydraulic compartments [19]. The scheme for the calculation of physicochemical iron removal from groundwater is shown in Fig. 2. The mathematical model assumes the presence of two forms of iron retained in the pore space of the packed bed. The clarification compartment is represented by equations describing, first, the transport,

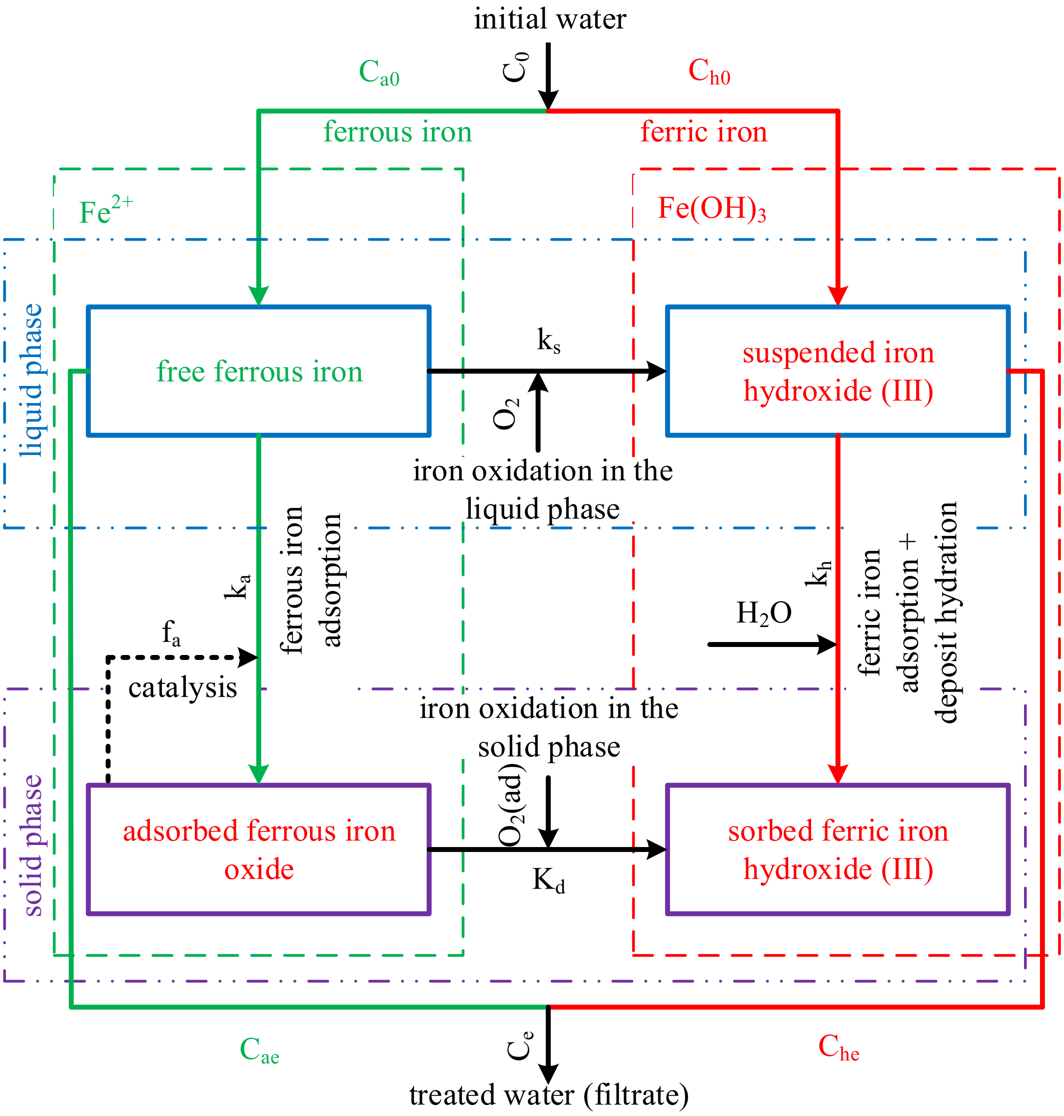

Fig. 2. Scheme of immobilization and transformation of iron forms at physicochemical iron removal from deep groundwater.

adsorption and oxidation of ferrous iron, secondly, the transport and sorption of ferric iron, and also boundary and initial conditions [17]. The key component of our proposed mass transfer model for the two forms of iron in filters of various design is a system of kinetic equations that takes into account the following.

- intensification of iron removal from water under the impact of the formed deposit;
- oxidation of ferrous iron predominantly in an adsorption form;
- the limitation of the sorption capacity, which leads with time to a noticeable decrease in the intensity of iron removal:

The method of aeration and filtration on granular filters has become widespread for the groundwater treatment [17]. The relatively high cost of excess iron removal from groundwater in Ukraine is largely due to the inefficient use of expensive filtering materials in specialized rapid filters [18]. Such filters are often operated impractically. Thus, the capital expenditure for the physicochemical removal of iron from artesian waters, which often meet the drinking water standards according to other environmental and sanitary indicators, can be determinative in assessing the price of water treatment [20]. Although, the operation costs also play a significant role.

It is well known that the optimization of the operation of any filtering plant consists of minimizing the total material and labor used in its construction, preparation for operation, and maintenance [21]. At the same time, it should be considered that iron removal filters operate under more difficult technological conditions than conventional filter – clarifiers for treating aqueous suspension due to the presence and the transformations of the two forms of iron, and most importantly, the progressive accumulation of the non-washable deposit [22,23]. Therefore, a special approach is required for calculating the filtration of water with a higher concentration of iron compounds. It allows for a quantitative analysis of the set of processes in the filter medium during both, a separate operating period and any of their sequences. When simulating physicochemical removal of iron, it is necessary to first set the initial concentration of the immobilized ferric iron, which is corrected considering the consolidation of the newly formed deposit at every calculation stage.

In general, the applied optimization of the operation of any water treatment filter should consist of choosing the least expensive process control algorithm from a variety of possible ones, ultimately reducing the water treatment cost. It is customary to operate with the concept of a representative filter run (is identified with the standard operation period) for rapid filter-clarifiers [24]. The filter control algorithm, during their prolonged operation, can be interpreted as a sequence of unified filter runs in the first approximation. Therefore, they have the same and the greatest duration considering the technological limitations. Abrasion of the packed bed elements (grains) is not taken into account; thus, it is often possible to significantly reduce the cost of the filter-clarifier operation by implementing such an algorithm in practice and sometimes prevent excessive deterioration of the filtrate quality.

The objectives of this work were.

- elaboration of the procedure of numerous consecutive technical and economic calculations of the operation of rapid filters under conditions of deposit consolidation, formation and accumulation of its non-washable component as a consequence;
- comparative analysis of technological process control algorithms used in the practice of physicochemical iron removal from deep groundwater and on its basis the development of recommendations on selection of the most economical algorithm.

2. Methodology

2.1. Technological optimization of the operation of a filter-clarifier

Technological optimization procedure which is commonly used at rapid filters in the separation of aqueous suspensions is based on two criteria of efficiency [25]. These criteria in symbolic form express the restrictions that must be imposed on the action of filters as clarifiers. Their observance should be constantly monitored. And above all, the concentration of residual disperse contamination in the filtrate C_e should not exceed the standard value C_*. Therefore, the next condition must be fulfilled as follows and determinate by Equation (1)

$$C_e \leq C_*. \tag{1}$$

The second requirement is determined by the rate mode. If the filtration rate is maintained constant due to special devices (regulators), then it is necessary to monitor the head losses in the packed bed Δh throughout the entire filter run. It is advisable to continue the filter operation only to the point where the specified losses have not reached the maximum allowable value Δh_*. Then the second criterion is formalized and determinate by Equation (2)

$$\Delta h \leq \Delta h_*. \tag{2}$$

The filter productivity gradually decreases due to unregulated filtration rate V. In this case, it is necessary to set a limit for such decrease based on economic considerations and determinate by Equation (3)

$$V \leq V_*. \tag{3}$$

From the sanitary, technical and economic standpoints of view, it is obvious that the productive operation of the filter can only be considered if conditions (1) and (2) or (3) are simultaneously met depending on the rate mode, (constant or variable rate).

Based on (1)-(3), it is advisable to introduce a number of technological times as follows:

- the time of the protective action of the filter bed t_p from the following equality as a partial case of ratio (1) is determinate by Equation (4)

$$C_e(t_p) = C_*; \tag{4}$$

- the time necessary to reach the maximum allowable head losses t_h from equality according to (2) is determinate by Equation (5)

$$\Delta h(t_h) = \Delta h_*; \tag{5}$$

- the time of allowable decrease in filter productivity t_V according to (3) is determinate by Equation (6)

$$V(t_V) = V_*. \tag{6}$$

Now the start time of the next backwashing of the filter (the duration of the filter run t_f) should be identified as the shortest of the indicated technological times. Formally it is determinate by Equation (7)

$$t_f = \min(t_p, t_h \ \ or \ \ t_V). \tag{7}$$

However, this approach is not sufficient for the technological optimization of the physicochemical removal of iron, because it helps to reduce operating costs. At the same time, capital costs, which play a special role in the economic analysis of the iron removal filter, are not taken into account. As a result, there is an urgent need for full-scale mathematical and technological modeling of such filters action. Therefore, it is necessary to analyze the changes in the filtration characteristics in detail (outlet concentration of total iron C_e, head losses in the packed bed, filtration rate) during at least the entire service life of the packed bed (the total time of the productive operation of the filter with one change of the filtering material t_s).

2.2. The optimization of filter operation during iron removal from deep groundwaters

The gel-like deposit that forms and distributes unevenly in the packed bed of a filter-clarifier does not consolidate. Therefore, almost all new deposit can be regularly removed due to a short-term intensive supply of treated water in the opposite direction. The technological process inside the iron removal filters proceeds fundamentally differently. Here, the progressive accumulation of the residual deposit from one filter run to another is clearly observed, which progresses from one to another filter run [23]. Its strength increases so much, due to the ongoing deep structurization with the formation of new stable chemical connections, that it is necessary to sharply increase the washout intensity and the volume of washout water in order to remove it. However, operating costs increase in an accelerated manner, which is economically disadvantageous. Therefore, the traditional approach to the operation optimization of the water treatment filters and substantiation of the design and technological parameters has to be significantly developed both in the engineering practice of iron removal and in its technological modeling. In fact, it is necessary to focus on the long-term control algorithm, which is implemented up to the complete exhaustion of the treated resource of the gradually contaminated filtering material. The design of an algorithm that can ensure the maximum service life of the filter medium can be the goal of such modeling in principle. It is logical that capital costs will be minimized in this way and, as a result, the cost of the treated water will be reduced significantly. But certainly, it is possible to achieve the maximum efficiency from the physicochemical removal of iron by filtration based only on the results of a special technical and economic analysis with the involvement of generalized (the reduced costs) and specialized (prices) economic indicators. As a rule, such information is difficult to access and insufficiently complete for mathematical modeling. Moreover, its reliability often raises doubts. The only real possibility to develop a rational filter control algorithm for the entire service life of the next filtering material change consists in attracting adequate mathematical models of the physicochemical removal of iron from groundwater and using effective methods of their solution. And only the application of correct solutions of the corresponding mathematical tasks to the entire sequence of filter runs, including the last run, (before the filtering material replacement) allows to estimate objectively the actual workability of the filter when removing excess iron and create a basis for subsequent technical and economic estimations.

The calculation method presented in Ref. [19] permits a significant variety both in the physicochemical state of the deep groundwater, which directly enters the medium, and in the filtering material before the next filter run. Fresh water in an aquifer that is deep-lying and is not exposed to the atmosphere contains iron exclusively in the ferrous form. Naturally, that the ratio between the contents of both forms of iron in the pumped groundwater significantly depends on the method and duration of such contact and the initial proportion of the ferric iron form can only increase and the ferrous iron form decrease respectively at the preparatory stage. From a technological point of view, the access of air to water can be simultaneously undesirable and desirable. Early interaction of groundwater with air, which accompanies their pumping, contributes to the deterioration of the technical condition of water intake equipment, even with its possible failure after long-term operation. On the contrary, water must be aerated to create favorable conditions for the oxidation of ferrous iron in the filter medium immediately before entering the filter. Here a practical question arises about the efficient depth of the aeration, since the cost of the treated water depends significantly on its solution. The practice of the physicochemical removal of iron indicates that simplified aeration is preferable at a comparatively low initial content of ferrous iron. It is simply implemented and, unlike forced aeration (using aerators), does not require additional and often very serious costs.

In fact, the deep groundwater supplied to the filter necessarily contains both forms of iron [26]. The ratio between them can vary widely in principle. As a basis for a comparison when estimating the degree of preliminary oxidation of the ferrous iron, (was initially in the fresh water of an isolated aquifer), it is advisable to take the sum of the initial volume fractions of ferrous iron C_{a0} and iron hydroxide C_{h0} (the previously oxidized part of the total amount $C_0 = C_{a0} + C_{h0}$ has concentration C_{h0} due to uncontrolled access of air to water and its special aeration). Then the entire range of possible situations with iron contamination of water immediately before filtration can be conveniently characterized by the normalized parameter $\Psi_0 = C_{a0} / (C_{a0} + C_{h0})$. In principle, Ψ_0 can vary within the maximum limits, i.e. from 0 to 1. However, this parameter is in a narrower range when using simplified aeration. It is important to note that the ratio Ψ_0 is not a calculated value, although it can be controlled. In fact, when modeling the iron removal process, it should be set based on the actual composition of the contamination at the filter inlet. It is especially important to regularly calculate the initial content of the immobilized iron with the greatest precision due to the accumulation of permissible computational errors. At this stage of calculations, it is justified to take the amount of ferrous iron adsorbed by the end of the previous stage as the initial amount after the corresponding recalculation. The amount of the deposit based on iron hydroxide is sharply reduced as a result of the medium washout. The residual amount of the deposit is simply set using the hydrodynamic resistance factor R_h. The indicated empirical coefficient characterizes the part of the non-washable deposit in the newly formed deposit and essentially depends on its age by definition [23]. Since the proportion of iron hydroxide in the deposit is stable, this coefficient can also be used to calculate the accumulation of the bound water and deposited ferric iron separately.

2.3. *Calculation of initial concentrations of immobilized ferrous and ferric iron*

The filter run number j is selected and considered separately from the numerous sequences of filter runs and the time count starts simultaneously with the start of the filter run. Then the calculation period will be $[0, t_{fj}]$. The volume fractions of the immobilized ferrous and ferric iron are assumed to be equal S_{aj}^0, S_{hj}^0 and are the same at any height due to intensive mixing and multiple collisions of the elements of the pseudo-fluidized packed bed as a result of its washout. The volume of the adsorbed ferrous iron will be in the bed with height L at the moment t $(t_{fj} \geq t > 0)$ as follows is determinate by Equation (8)

$$\int_0^L S_{aj}(z,t)dz. \tag{8}$$

2.3.1. *Iron hydroxide is also additionally immobilized in it, namely*

$$W_j(t) = \int_0^L \left[S_{hj}(z,t) - S_{hj}^o\right] dz.$$

The next hydroxide amount will be added after the interval Δt.

$$\Delta W_j = W_j(t+\Delta t) - W_j(t) = \frac{\partial W_j}{\partial t}\Delta t.$$

The age of a given portion of the deposited ferric iron immediately before the washout j will determinate by Equation (9)

$$t_{aj}(t) = t_{fj} - t. \tag{9}$$

The residual of this portion will remain in the medium after the washout is determinate by Equation (10)

$$\frac{\partial}{\partial t}W_j(t)\ R_h\left(t_{fj} - t\right)\Delta t. \tag{10}$$

The expression (10) must be integrated over time in the range from 0 to t_{fj} to determine the total amount of the new deposited hydroxide remaining after the washout. Then the residual concentration of hydroxide (initial for the filter run $j+1$) will determinate by Equation (11)

$$S_{h,j+1}^o = S_{h\,j}^o + \frac{1}{L}\int_0^{t_{fj}} \frac{\partial}{\partial t}W_j(t) \cdot R_h\left(t_{fj} - t\right)\, dt. \tag{11}$$

The expression for the new initial value of the concentration of the iron hydroxide (filter run $j+1$) has the following dimensionless form

$$S_{h,j+1}^o = S_{hj}^o + \frac{R_h(0)W_j\left(t_{fj}\right)}{L} - \frac{1}{L}\int_0^{t_{fj}} W_j(t)\frac{d}{dt}R_h\left(t_{fj} - t\right)dt.$$

The concentration of the iron hydroxide (filter run $j+1$) has the dimensionless form of the expression for the new initial value is determinate by Equation (12)

$$\overline{S}_{h,j+1}^o = \overline{S}_{hj}^o + R_h(0)\overline{W}_j\left(\bar{t}_{fj}\right) - \int_0^{\bar{t}_{fj}} \overline{W}_j(\bar{t})\frac{d}{d\bar{t}}R_h\left(\bar{t}_{fj} - \bar{t}\right)d\bar{t}. \tag{12}$$

Here $\overline{S}^o_{hj} = \frac{S^o_{hj}}{n_0C_0}$, $\overline{t} = \frac{Vt}{n_0L}$, $\overline{W}_j = \int\limits_0^1 [\overline{S}_{hj}(\overline{z},\overline{t}) - \overline{S}^o_{hj}]\, d\overline{z}$, $\overline{S}_h = \frac{S_h}{n_0C_0}$.

As the result of the supply of both forms of iron into the filter being even over time, the smoothness and almost linear nature of the changes in $\overline{W}_j$, it is possible, in order to simplify, to use the average age $0.5\overline{t}_{fj}$ for the accumulated deposit during the filter run j.

$$R_h(\overline{t}_{fj} - \overline{t}) \approx R_h(0.5\overline{t}_{fj}).$$

We substitute the exact expression for an approximate expression with minimal errors. Then

$$\overline{S}^o_{h,j+1} = \overline{S}^o_{hj} + R_h(0.5\overline{t}_{fj}) \int\limits_0^1 \left[\overline{S}_{hj}(\overline{z},\overline{t}_{fj}) - \overline{S}^0_{hj}\right] d\overline{z}.$$

Finally, it is determinate by Equation (13)

$$\overline{S}^o_{h,j+1} = \overline{S}^o_{hj}\left[1 - R_h(0.5\overline{t}_{fj})\right] + R_h(0.5\overline{t}_{fj}) \int\limits_0^1 \overline{S}_{hj}(\overline{z},\overline{t}_{fj})\, d\overline{z}. \tag{13}$$

At last, due to the redistribution in the pseudo-fluidized medium of the filtering material of the ferrous iron, that was adsorbed by the end of the filter run j (we neglect desorption), the relative concentration of ferrous iron at the beginning of the filter run $j+1$ according to (9) will determinate by Equation (14)

$$\overline{S}^0_{a,j+1} = \int\limits_0^1 \overline{S}_{aj}(\overline{z},\overline{t}_{fj})\, d\overline{z}. \tag{14}$$

2.4. Calculation scheme

The calculation scheme involves a step-by-step implementation of a large amount of calculations. The first filter run is the single calculation stage for which we accept $S^0_a = S^0_h = 0$ due to the beginning of the operation of a new packed bed. The distribution functions are specified at the end of this stage $S_a(z, t_{f1}), S_h(z, t_{f1}), S_d(z, t_{f1})$ (S_d – is the volumetric deposit concentration, i.e. its specific volume). It is necessary to preliminarily calculate the initial distribution functions $S^0_{a2}(z), S^0_{h2}(z)$ in order to continue the calculations at the next stage (the second filter run), based on the data of the previous calculation stage. The age and strength of the deposit, the washout efficiency, the redistribution of the adsorbed ferrous iron and the deposited ferric iron along the medium height should be taken into account when determining them. Thus, it is reasonable to take the following relative constant values in accordance with (12), (14) or simplified (13) it is determinate by Equation (15)

$$\overline{S}^0_{a2} = \int\limits_0^1 \overline{S}_{a1}(\overline{z},\overline{t}_{f1})\, d\overline{z},\ \overline{S}^0_{h2} = R_h(0.5\overline{t}_{f1}) \int\limits_0^1 \overline{S}_{h1}(\overline{z},\overline{t}_{f1})\, d\overline{z}. \tag{15}$$

As is known [16], the proportion of iron hydroxide in the deposit can be characterized by the coefficient of the physicochemical state γ, which depends on the concentration of the deposited hydroxide S_h. Note that it is reasonable to use its average value γ_{av} in the applied calculations due to the smooth and almost linear nature of the decrease with increasing S_h. The calculation expressions arising from its solution are primarily intended to predict their spatiotemporal changes since the basic task is formulated relative to the volume fractions of the ferrous iron in the adsorbed (S_a), dissolved (C_a) states and similarly to concentrations of the deposited (S_h) and dissolved (C_h) hydroxide. The deposit dynamics is easy to follow because the aforementioned coefficient is being used. Therefore, the first portion of the non-washable deposit is characterized by a relatively constant volume fraction along the height (specific volume) by Equation (16)

$$\Delta\overline{S}_{d2} = \gamma\left(\overline{S}^0_{h2}\right)\overline{S}^0_{h2}. \tag{16}$$

It should be noted that it is necessary to take the same value γ (or γ_{av}) for both the fresh and non-washable deposits.

In fact, the entirety of the major calculations of the filtration characteristics, which has to be performed during a detailed technical and economic analysis of the operation of the iron removal filter, is conditionally divided into N stages (by the number of the filter runs). Two approaches to the choice of the duration of these stages are implemented in practice, these are essentially the two main algorithms of the iron removal control. The principle of establishing the characteristic duration t_f becomes of key importance in the theoretical substantiation of the control algorithm. It is necessary to apply the technological optimization procedure, which is standard for the filter-clarifiers, at every calculation stage if we strive to maximally reduce the cost of the filter operation. The treatment potential at the end of every filter run is fully utilized with this approach, which is the basis of the irregular algorithm. Thus, calculations at every stage of the control algorithm using a calculation step unevenly distributed over time $(t_{fj} > t_{f\,j+1})$ are carried out as long as both criterion conditions are satisfied, namely, (1) and (2) in the case of the constant rate mode ($V = const$). In fact, the duration of the filter run number $j(N \geq j \geq 1)$ t_{fj} is calculated for given and corresponding initial concentrations S^0_{aj}, S^0_{hj}. At the same time, the final distribution functions $S_{aj}(z, t_{fj}), S_{hj}(z, t_{fj})$ are concretized using already known value t_{fj}. Firstly, the indicated profiles of both concentrations serve as the basis for determining the initial values $S^0_{a,j+1}, S^0_{h,j+1}$ for the subsequent filter run number $j+1$. They are calculated, assuming full mixing of the set of the structural elements of the medium, according to (12) or (13) and (14). The fact that the duration t_{fj} is reduced to a value that is less than the minimum allowable t_* experimentally established (according to the formally accepted assumption assuming the N filter runs can be performed in time t_s, it should be $j = N$ in the specified duration, so that $t_{fN} > t_* > t_{f,N+1}$), indicates the functional unsuitability of the contaminated medium and the need for its immediate replacement.

The additional amount of the deposit that remains in the medium and is distributed in it evenly after a sufficiently intensive washout number j is at the set value $\overline{S}^0_{h\,j}$. The corresponding relative concentration $\Delta\overline{S}_{dj}$ is calculated using the formula to generalize (16)

$$\Delta\overline{S}_{dj} = \gamma\left(\overline{S}^0_{h\,j}\right)\overline{S}^0_{hj} - \sum\nolimits_{k=1}^{j-1}\Delta\overline{S}_{dk}.$$

However, it is extremely difficult to constantly control the technological process and automate it in the case of the implementation of the irregular algorithm, which allows to maximally prolongate the filter operation.

It is technically much easier to organize a continuous operation of the filter at a fixed duration of the filter run. Here, instead of different N and previously unknown values t_{fj}, it is enough to substantiate and then operate with a single value t_f. Preliminarily, it can only be approved that the specified value should be much less t_{f1} than that related to the irregular algorithm (with decreasing t_{fj}), and the final calculated values C_e and Δh should be approximately equal to C_*, Δh_* for the final filter run ($j = N$), and at the same time $t_{fN} \approx t_f$, where t_{fN} is determined according to the above optimization procedure. The problem here is to establish the appropriate initial values S^0_{aN}, S^0_{hN}, which requires a complex of calculations in full for the filter runs from the first run to run number $j - 1$. The number of calculations can be significantly reduced if we begin to control the quality of the filtrate and the head losses in a packed bed after a sufficiently long operation of the filter. The combined algorithm was considered in addition to the main algorithms. At the same time, two sequences of filter run with different fixed durations and fit into the service life t_s.

The basis for our developed method of technical and economic analysis of physicochemical iron removal from deep groundwater was a nonstationary nonlinear mathematical model consisting of three interconnected compartments, as well as its exact solution [19]. In order to provide the model with the initial information in full, comprehensive experimental studies were carried out in laboratory and production conditions [[23,26]]. A procedure of continuous step-by-step calculations was organized and implemented using Mathcad to establish technological parameters and economic indicators with a focus on the reduced costs during the service life of the filtering material change. The mentioned procedure allows to analyze operatively and in a dialog mode the impact of physicochemical conditions at the boundaries and inside the bed on the quality of water treatment and mechanical energy resource of the filter, to substantiate the economic expediency of application of modern control algorithms and to optimize them.

3. Results and discussion

3.1. Technical and economic analysis

The control time T sets for a generalized economic analysis of the costs of the filtration of deep groundwaters. It includes both the productive time (the actual filter operation) and unproductive time (spent on all washouts).

The basic equation for the technical and economic analysis in general view will be determinate by Equation (17)

$$CC + OC = V\mathrm{T}\Omega_F P_W, \tag{17}$$

where CC, OC are the capital and operation costs respectively); Ω_F is the medium surface area; P_W is the cost of the treated water per each volume unit.

The part of the costs that was spent on expensive filter material is separated from the capital costs, it is determinate by Equation (18)

$$CC = \Omega_F L P_F \frac{\mathrm{T}}{t_S} + \Delta CC, \tag{18}$$

where ΔCC are all other points of the capital costs (automation equipment, pumps, aerators, etc.), P_F is the cost of a unit volume of the filtering material and the cost of its replacement. Also, in the second term of equation (17), the costs of regular washouts are considered separately, namely it is determinate by Equation (19)

$$OC = N_{\mathrm{T}} P_{BW} + \Delta OC. \tag{19}$$

Here N_{T} is the number of filter runs per time T, P_{BW} is the cost of one washout.

Taking into account (18), (19), equation (17) can be presented as follows and determinate by Equation (20)

$$L\Omega_F P_F \frac{\mathrm{T}}{t_s} + N_T P_{BW} = V\mathrm{T}\Omega_F P_W - \Delta CC - \Delta OC, \tag{20}$$

and after dividing both parts of equation (20) by $V\mathrm{T}\Omega_F$ we obtain as following by Equation (21)

$$\frac{LP_F}{Vt_S} + \frac{N_\mathrm{T}}{\mathrm{T}}\frac{P_{BW}}{V\Omega_F} = P_W - \frac{\Delta CC + \Delta OC}{V\mathrm{T}\Omega_F}. \tag{21}$$

The relative time is introduced to generalize the results of the subsequent calculations. Therefore, $\bar{t}_s = \frac{Vt_s}{n_0 L}$, $\overline{T} = \frac{V\mathrm{T}}{n_0 L}$. Then equation (21) will be determinate by Equation (22)

$$\frac{P_F}{\bar{t}_s} + \frac{N_\mathrm{T}}{\overline{\mathrm{T}}}\frac{P_{BW}}{L\Omega_F} = n_0\left(P_W - \frac{\Delta CC + \Delta OC}{\overline{\mathrm{T}}L\Omega_F}\right). \tag{22}$$

In the case of the second algorithm $(t_{fj} = t_f)$ equation (22) transforms in the following and determinate by Equation (23)

$$\frac{P_F}{\bar{t}_s} + \frac{P_{BW}}{L\Omega_F \bar{t}_f} = E_W = n_0\left(P_W - \frac{\Delta CC + \Delta OC}{L\Omega_F \overline{\mathrm{T}}}\right), \overrightarrow{t}_s = N\bar{t}_f = \sum_{j=1}^{N} \bar{t}_{fj}. \tag{23}$$

Thus, the reduced costs of the treated water *RC* depend on the time parameters $\bar{t}_s$, $\bar{t}_f$ in accordance with (23), and consequently on the control algorithm. It is logical that the choice of the algorithm here is the final goal of the technical and economic analysis that results in $RC = \min$. In fact, such values should be specified as $\bar{t}_s$ and $\bar{t}_{f,av} = \overline{\mathrm{T}}/N_\mathrm{T}$ (or $\bar{t}_f$), at which it will be possible to minimize the right-hand sides of equations (22) and (23).

Studying the influence of three factors on *RC* that have economic and technological meanings became the goal of a detailed technical and economic analysis. First, the value *RC* was calculated depending on the initial ratio of the concentrations of two iron forms Ψ_0. This ratio is directly related to preliminary aeration (forced, simplified), which significantly affects the cost of water treatment. Secondly, three control algorithms associated with *RC* are the irregular (with an even calculation step), regular (with an uneven calculation step, so that $t_{fj} = t_{f\,j+1} = t_f$) and combined (with different calculation steps, $t_{fI} > t_{fII}$). Thirdly, the efficiency of iron removal at different degree of groundwater contamination characterized by the sum $C_0 = C_{a0} + C_{h0}$ was estimated.

Input data array necessary for the technological modeling was prepared in full, primarily due to a set of experimental studies at laboratory and industrial plants. These studies were planned based on the fundamental non-linear non-stationary mathematical model of the physicochemical removal of iron from groundwater. The mathematical processing of the regime information, which was obtained during the experiments on the above-mentioned plants, made it possible to establish the characteristic values of all model coefficients. They are presented in the articles [16–18]. Also, the successful experience of long-term operation of iron removal plants of various designs and filtration rates was involved. The specified array was conditionally divided into three groups of parameters depending on the goal application. The empirical coefficients which fully provide an adequate description of the phenomenology of non-biological removal of iron belong to the most numerous groups. The tasks set by us for the technological modeling made it possible to initially fix the values of the indicated coefficients, then calculate the dimensionless analogs, which were involved without changes in all calculations. The second group also included stable technological-criteria constants $\overline{C}_*$; $\Delta\overline{h}_* = 6$; $\bar{t}_* = 100$. The dimensionless values $\overline{C}_* = C_*/C_0$ depended on the total amount of iron at the inlet to the medium. Thus, if $C_0 = 1\ mg/dm^3$, then $\overline{C}_* = 0.2$. The variation of the parameters of the third group within a wide range, corresponding to both normal and extreme technological conditions, made it possible to objectively and comprehensively assess the practical possibilities of the physicochemical iron removal. The value Ψ_0 was changed continuously or discretely (the characteristics of the contamination composition), C_0 (contamination rate), t_f (technological time interval).

The quantitative analysis was conducted primarily to illustrate the effectiveness of the proposed method of the technical and economic optimization of the technology of iron removal from groundwater by filtration. The results of the analysis are significant and can contribute to the rational choice of the technological parameters under similar conditions, since real initial data obtained by experimental methods on pilot plants and operating filters with widely used filtering material were utilized. It is obvious that the effectiveness of the operating procedure significantly depends on the filter operation algorithm. The three algorithms described above were compared to determine the most cost-effective option. At the same time, great importance was attached to the possibility of implementing the algorithm with minimal labor costs, i.e. filter automation. The corresponding expense item was not taken into account directly when determining the reduced costs due to the complexity of its cost estimation, but it should be considered when making a final decision on the method and means of control.

Therefore, the main efforts were directed to studying the effectiveness of the regular algorithm (I), which is easily automated unlike the other two algorithms. To substantiate a constant operating time interval t_f (an analogue of the filter run in deep-bed filtration of aqueous suspensions) as the most important characteristic of this algorithm, it was varied discretely or continuously within such a framework that the filter operation was ensured over a certain sequence of marked intervals.

The specifics of using the irregular algorithm (II), the traditional algorithm for filter-clarifiers, is that the amount of non-washable deposit increases under the conditions of the physicochemical removal of iron and the adsorption capacity of the packed bed decreases with every filter run. Therefore, it is impossible to unify the calculations of water treatment by filtration in this case which necessitates the determination the corresponding duration t_{fj} at every (j) stage (a separate operating period). As a result, a numerous sequence of decreasing relative values $\bar{t}_{fj}$ $(j = 1, 2, \ldots)$ is calculated.

The combined algorithm (III), which can be considered as a combination of the first two algorithms, was analyzed fragmentarily due to significant difficulties in automating the algorithm II. Now the every next value t_{fq} was maintained for a number of operating intervals and until either the head losses in the bed or the contamination concentration at its outlet did not exceed the limit values Δh_* and C_* respectively. Then the accepted value $\bar{t}_{fq}$ immediately decreased by 100 units and the procedure for calculating the desired characteristics at the new value $\bar{t}_{f,q+1}$ was repeatedly duplicated, starting from the last calculation interval and up to the next violation of conditions (1) and (2). All predictive, technical and economic calculations were completed if in the case of the algorithm II every next value is $\bar{t}_{fj}$, and in the case of the algorithm III the last value $\bar{t}_{fq}$ (obviously that $j \gg q$), they did not turn out to be less than the minimal value allowed by regulatory documents (corresponds to the dimensional value $t_f = 8$ hours).

The total time of the effective operation of the filter material used for iron removal before its replacement primarily is of special interest due to its high cost. In general, the service life T_f of the medium depends on the properties of its material, filtration conditions and the way the filter is operated. In the first series of examples, the subject of calculations is just the relative service life $\overline{T}_f$ of a bed of a given height and well-studied filter materials (polystyrene foam, zeolite, crushed granite) under varying conditions (Ψ_0, C_0) and filter operation in accordance with the three algorithms above. In this case, it is necessary to focus attention on the regular algorithm according to which the desired value $\overline{T}_f$ demonstrates the particular sensitivity. Discrete or continuous changes (several times) in the interval t_f caused disproportionately larger (tens of times) changes in $\overline{T}_f$. The longest service life was obtained in the examples at $\bar{t}_f = 100,\ \Psi_0 = C_0 = 1$ and served as a scale for all other values of $\overline{T}_f$.

Fig. 3 is especially illustrative, since it shows the importance of choosing the right operation algorithm for the service life of one change of the filtering material. Here, a typical (moderate) initial level of water contamination is assumed $(C_0 = 1mg/dm^3)$ and any composition of the contamination is allowed $(1 \geq \Psi_0 \geq 0)$. Fig. 3 illustrates, first of all, the impact of the ratio between two forms of iron in the initial water on the efficiency of the packed bed. If you want to achieve a longer service life, first, you should minimize the initial amount of ferric iron as much as possible and, secondly, ensure the same length of the operating periods. At the same time, it should remember that changes in $\bar{t}_f$ lead approximately to changes in $\overline{T}_f$ in the inverse proportion.

The initial content of iron significantly affects the period $\overline{T}_f$, as evidenced by Fig. 4. The dependence graphs of $\overline{T}_f$ on C_0 correspond to the limiting case $\Psi_0 = 1$, when the water entering the granular medium contains only ferrous iron, and also to different fixed values of $\bar{t}_f$ (algorithm I). Almost the same reduction in $\overline{T}_f$ is observed with an increase in C_0 at least in the range of $2 \geq C_0 \geq 1$. It makes sense to discuss the service life only for short operating intervals with severe contamination of the water supplied to the filter and its operation according to the regular algorithm. In particular, the filter is generally unable to reduce the inlet concentration to the maximal allowable C_* at $C_0 = 3\ mg/dm^3$ and $\bar{t}_f \geq 300$. Therefore, we can formally consider $\overline{T}_f = 0$. Unlike the regular algorithm, the irregular algorithm II contributes to the long-term operation of the filter material change due to the maximal exhaustion of the treating resource during every filter run also at $C_0 = 3\ mg/dm^3$. Moreover, an increase in $\overline{T}_f$ should be noted as the groundwater contamination by ferrous iron increases starting from the concentration of $2\ mg/dm^3$.

However, the long service life of the medium does not mean low total costs for the physicochemical iron removal. Therefore, it is necessary to conduct a complete joint technical and economic analysis of its functioning in the development of final recommendations for optimal filter operation. It is essential to consider the capital costs together with the operating costs and the goal of the technical and economic calculations should be the reduced costs for treating a unit volume of groundwater. Figs. 5 and 6 present the calculations data of the capital (CC), operating (OC) and, as a result, reduced costs (RC) at $C_0 = 1.5\ mg/dm^3$ in order to visually compare the contribution to the total costs of both components (CC and OC). Specifically, Fig. 5 shows the contamination composition parameter Ψ_0, which serves as an argument and makes it possible to visually assess its impact on the costs inventory when using different filter operation methods. Three sets of curves are shown here, the first set corresponds to the algorithm I (curves 1–3) – at $\bar{t}_f = 600$, the second set corresponds to the algorithm II (curves 4–6). Finally, the third set corresponds to the algorithm III and is composed of curves

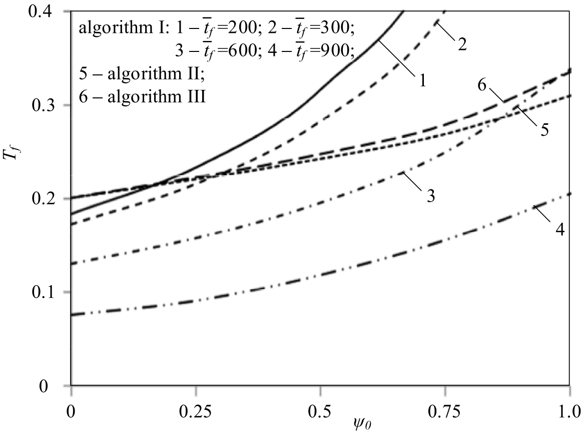

Fig. 3. Dependence $\overline{T}_f(\psi_0)$ at $C_0 = 1\ mg/dm^3$.

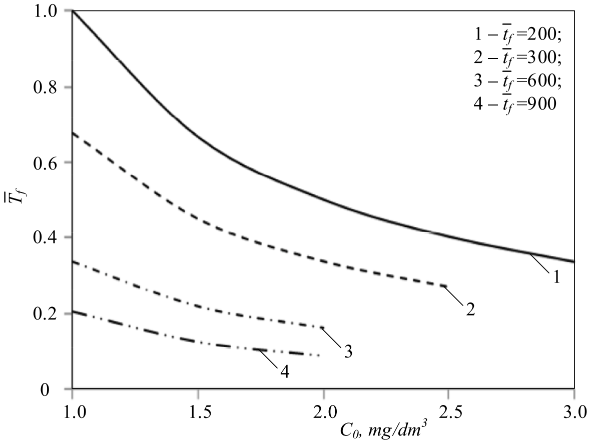

Fig. 4. Dependence $\overline{T}_f(C_0)$ at $\psi_0 = 1$, algorithm I.

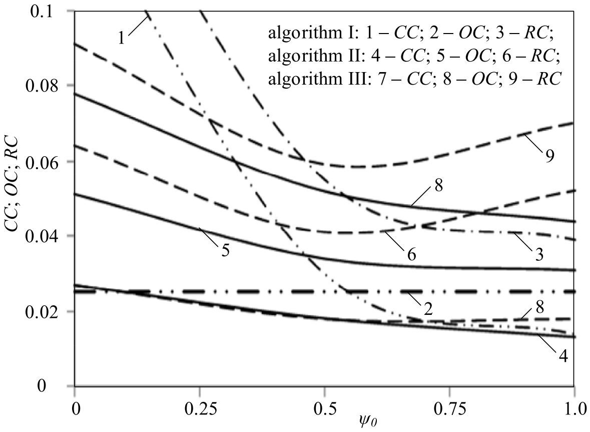

Fig. 5. Dependences $CC(\psi_0), OC(\psi_0), RC(\psi_0)$ at $C_0 = 1.5\ mg/dm^3$.

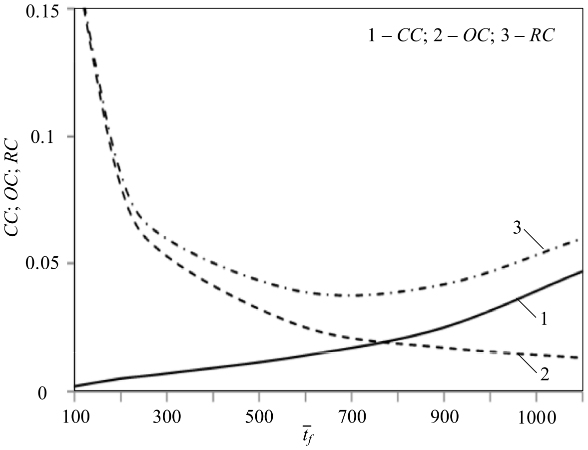

Fig. 6. Dependences $CC(\psi_0), OC(\psi_0), RC(\psi_0)$ at $\Psi_0 = 1, 0$, $C_0 = 1.5\ mg/dm^3$, algorithm I.

7–9. Fig. 6 refers exclusively to the regular algorithm and demonstrates the consequences of continuously varying the operating interval $\bar{t}_f$ for different types of costs. Here it is appropriate to note that the operating costs of rapid filters for water treatment in general are mainly associated with their regeneration. The amount of backwashing water is proportional to the number of the operating intervals in the service life with standard backwashing of the filter medium with a fixed volume of pure water to remove the iron deposit. As a consequence, the operating and capital costs at small and large values of $\bar{t}_f$ respectively clearly prevail. At the same time, they are so significant that the *RC* turn out to be significantly greater than the optimal value, at least in the examples calculated here. All subsequent results refer exclusively to *RC* as to a function of Ψ_0, C_0, t_f because in the joint technical and economic analysis the values *CC* and *OC* play a subordinate role and are aimed at establishing the reduced costs precisely.

The oxygen in groundwater with a high content of ferrous iron can significantly change the ratio between it and ferric iron in favor of the ferric iron [17,18]. Thus, the formation of a ferruginous deposit in the bed and, as a result, an increase in the consumption of mechanical energy are accelerated and ultimately its service life is reduced. As a first approximation, the effect of oxygen on the technological process and the efficiency of the filter can be taken into account by selecting a suitable value Ψ_0. In the third series of examples, this factor is reflected to the maximum possible extend based on its continuous variability from 0 to 1. The results of calculating the reduced costs *RC* depending on Ψ_0 are summarized in Figs. 7 and 8 and correspond to all three operation algorithms. Five characteristic values $\bar{t}_f$ are chosen in the case of the regular algorithm. The costs *RC* increase significantly as Ψ_0 decreases when water contamination at the inlet to the filter is moderate (Fig. 7). If we choose the minimal $(\Psi_0 = 1)$ values of *RC* as reference values for comparison, then the maximal increase is estimated at about 23.5% (algorithm II), 10.9% (algorithm III), 22 … 40% or more (algorithm I). The sensitivity of the costs *RC* to Ψ_0 increases multiple times when the level of the initial contamination is doubled (Fig. 8). Specifically, the pre-oxidation of all ferrous iron will cause an increase in *RC* by 4.4 times when the algorithm II is implemented, in 4.3 times with the algorithm III, in 1.54 times with the algorithm I $(\bar{t}_f = 200)$. It is important to note that the calculated curves in Figs. 7 and 8, corresponding to the algorithms II and III and also to the values $\bar{t}_f$ (algorithm I), are very different. This fact highlights the significance of the value C_0 for the filter operation. The following series of examples just allows to directly assess the significance of the initial contamination (C_0) for the economics of the physicochemical removal of iron.

The concentration of iron mainly in the ferrous form varies in the deep groundwaters of Ukraine in a very wide range – from $1\ mg/dm^3$ to $3\ mg/dm^3$, although there are regions with iron concentrations over $20\ mg/dm^3$. The value C_0 is characterized by significant variability and within not only geological and geographical regions, but also individual geological massifs. The choice of the method, technical means and technological scheme of iron removal depends on the level of contamination of groundwater with iron compounds. Therefore, the economic basis for the practicability (or non-practicability) of using the selected three algorithms for slightly contaminated and highly contaminated waters with an admixture of different composition was in the focus of attention when we considered the theoretical methods of the physicochemical water treatment at rapid filters. The reduced costs only served as an indicator of the economic efficiency of measures needed to prepare the filter for functioning and being operated. A series of figures is calculated, representing in graphical form the functional relationship between *RC* and C_0. The argument (C_0) changed continuously from $1\ mg/dm^3$ to $3\ mg/dm^3$. The detailed calculations of *RC* covered all the basic values Ψ_0, three algorithms and four values of $\bar{t}_f$ for the algorithm I, considering the practical importance of $E_w(C_0)$. It should be noted that groundwater treatment became more expensive with higher initial contamination in all examples, regardless of the algorithm and contamination composition. However, the nature of the impact of the total concentration C_0 on *RC* may change significantly in response to the variability of the degree and composition of contamination and also the values of $\bar{t}_f$ in the case of regular process operation. The results of the detailed numerical and analytical calculations of *RC*, which are figured in Figs. 9–11, allow us to evaluate the way C_0 impacts the economy of the removal of iron compounds from groundwater under real various physical and technological conditions of filtration. Also, the array of data obtained in this way is summarized in Table 1, where the form of limiting the processing procedure is specified along with the actual values of *RC* namely based on the head losses (t_h) or filtrate contamination (t_p). Factually, the costs *RC* increase smoothly and in a linear manner as C_0 increases when the total level of iron in water $(2 \geq C_0 \geq 1\text{Мг}/\text{дМ}^3)$ is moderate, its predominant initial content is in the ferrous form $(\Psi_0 \geq 0.5)$ and time intervals $\bar{t}_f$ are relatively short. The behavior of the graphs of the dependence $RC(C_0)$ changes drastically with severe contamination $(3 \geq C_0 > 2\ mg/dm^3)$, a higher initial content of the oxide form $(\Psi_0 < 0.5)$, also extending the regular time of continuous operation of the filter (algorithm I). The significant non-linearity shown on the calculated curves is explained by the

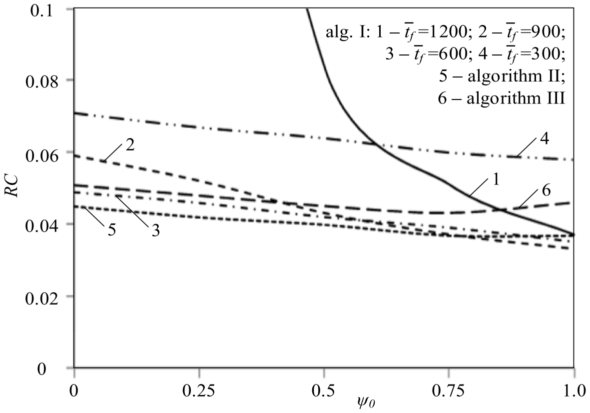

Fig. 7. Dependence $RC(\Psi_0)$ at $C_0 = 1\ mg/dm^3$.

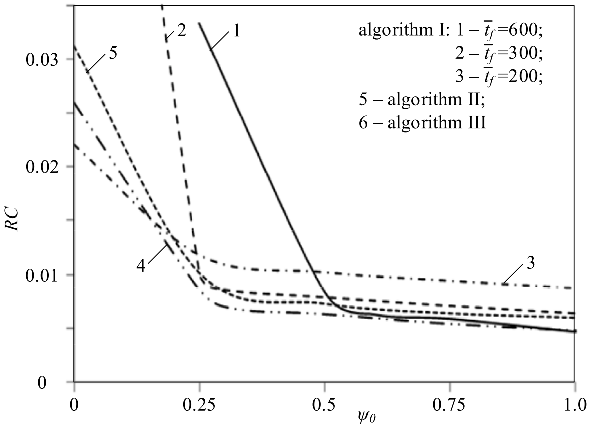

Fig. 8. Dependence $RC(\Psi_0)$ at $C_0 = 2$ mg/dm^3.

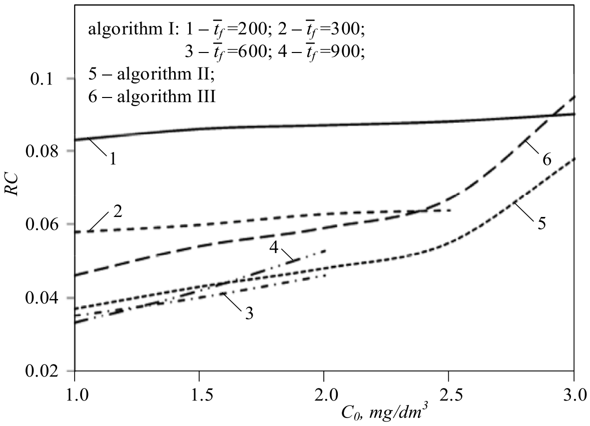

Fig. 9. Dependence $RC(C_0)$ at $\Psi_0 = 1$.

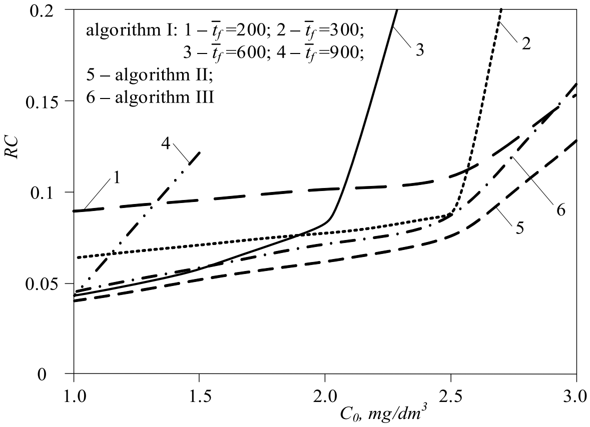

Fig. 10. Dependence $RC(C_0)$ at $\Psi_0 = 0.5$.

filtration conditions being close to becoming critical, which from a physical point of view means either accelerated accumulation of a deposit in the packed bed or accelerated a decrease in its protective ability. The value of RC will grow uncontrollably if you continue to hypothetically increase C_0, t_f and decrease Ψ_0. This can be interpreted in practice as a crisis of iron removal by filtration. In other words, the filter is completely unable to function productively and efficiently (see Table 2).

In order to still achieve the desired result, namely, treatment of the required volume of water of a standard quality in a given time, it

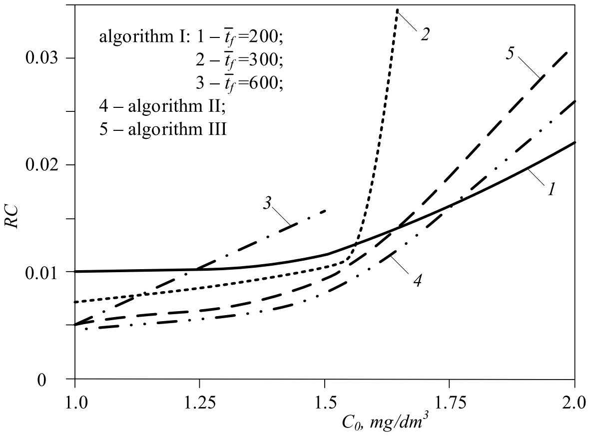

Fig. 11. Dependence $RC(C_0)$ at $\Psi_0 = 0$.

Table 1
Values of *RC* and nature of the technological process limitation (t_h *or* t_p) for the operation algorithm I.

ψ_0	$\bar{t}_f$					
	100	200	300	600	900	1200
$C_0 = 1$ mg/dm^3						
0	0.188 (t_h)	0.098 (t_h)	0.071 (t_h)	0.049 (t_h)	0.059 (t_h)	1 (t_h)
0.5	0.18 (t_h)	0.09 (t_h)	0.064 (t_h)	0.042 (t_h)	0.043 (t_h)	0.084 (t_h)
1	0.171 (t_h)	0.083 (t_h)	0.058 (t_h)	0.035 (t_h)	0.033 (t_h)	0.037 (t_h)
$C_0 = 1.5$ mg/dm^3						
0	0.199 (t_p)	0.113 (t_p)	0.093 (t_p)	0.157 (t_p)	–	–
0.5	0.184 (t_h)	0.096 (t_h)	0.071 (t_h)	0.057 (t_h)	0.122 (t_h)	–
1	0.172 (t_h)	0.086 (t_h)	0.06 (t_h)	0.04 (t_h)	0.042 (t_h)	0.06 (t_h)
$C_0 = 2$ mg/dm^3						
0	0.252 (t_p)	0.219 (t_p)	0.973 (t_p)	–	–	–
0.5	0.189 (t_h)	0.102 (t_h)	0.078 (t_p)	0.083 (t_p)	–	–
1	0.173 (t_h)	0.087 (t_h)	0.063 (t_h)	0.046 (t_h)	0.053 (t_h)	0.093 (t_h)
$C_0 = 2.5$ mg/dm^3						
0	–	–	–	–	–	–
0.5	0.195 (t_h)	0.108 (t_h)	0.088 (t_p)	0.311 (t_p)	–	–
1	0.173 (t_h)	0.088 (t_h)	0.064 (t_h)	–	–	–
$C_0 = 3$ mg/dm^3						
0	–	–	–	–	–	–
0.5	0.212 (t_p)	0.154 (t_p)	0.431 (t_p)	–	–	–
1	0.175 (t_h)	0.09 (t_h)	–	–	–	–

Table 2
Values of *RC* and nature of the technological process limitation (t_h or t_p) for the operation algorithm II и III

Algorithm	ψ_0		
	0	0.5	1
$C_0 = 1$ mg/dm^3			
II	0.045 (t_h)	0.04 (t_h)	0.037 (t_h)
III	0.051 (t_h)	0.045 (t_h)	0.046 (t_h)
$C_0 = 1.5$ mg/dm^3			
II	0.076 (t_p)	0.052 (t_h)	0.043 (t_h)
III	0.09 (t_p)	0.059 (t_h)	0.053 (t_h)
$C_0 = 2$ mg/dm^3			
II	0.26 (t_p)	0.063 (t_h)	0.048 (t_h)
III	0.313 (t_p)	0.072 (t_h)	0.059 (t_h)
$C_0 = 2.5$ mg/dm^3			
II	–	0.076 (t_p/t_h)	0.055 (t_p/t_h)
III	–	0.088 (t_p/t_h)	0.067 (t_h)
$C_0 = 3$ mg/dm^3			
II	–	0.129 (t_p)	0.078 (t_p/t_h)
III	–	0.16 (t_p)	0.095 (t_h)

is necessary to reduce the duration of filter runs, or treat low-quality filtrate further, or improve the design of the filter.

The filter runs are limited first by the time of the protective action of the bed t_p (limited by the quality of the filtrate) and then by t_h (by head losses) at initial iron concentrations of $2.5 - 3\ mg/dm^3$ and $\Psi_0 = 1$ for the operation algorithm II (Table 2). Similar results were obtained for the algorithms II and III at initial iron concentration of $2.5\ mg/dm^3$ and $\Psi_0 = 0.5$. A similar change in the nature of the limitation of the technological process during the operation of one replacement of the medium also takes place if the algorithm III is implemented and $\Psi_0 = 0.5$. The duration of the filter runs is initially determined by the outlet concentration of iron in the oxide form predominantly, which rapidly increases with time due to the relatively low clogging and adsorption ability of the filter material in relation to ferric iron and its comparatively high initial content. The progressive accumulation of ferruginous deposit causes a fundamental change in the assessment of the filter's functionality after a significant amount of time, from a technological point of view. Now, the consumption of mechanical energy for filtration as a result of increased contamination of the porous medium increases so much that the time t_h decreases in comparison to t_p despite a significant reduction in the absorption resource of the medium and accordingly the process time t_p.

An unusual situation develops at the implementation of the algorithm I in relation to strongly contaminated groundwater. In the cases considered in detail $C_0 = 2.5\ mg/dm^3$ and $\bar{t}_f = 600$, as well as $C_0 = 3\ mg/dm^3$, $\bar{t}_f = 300$ and in the presence of only one form of contamination initially and already during the first operating interval, the maximum allowable head losses in the bed and the concentration of iron in the filtrate are exceeded. Thus, the filter is initially unable to provide the required result in the given technological conditions. At the same time, it can operate normally for a short period of time with an equal initial content of both forms, – in the first case for 70 intervals (42000 units), in the second case for 107 intervals (32100) with an equal initial content of both forms. The operability of the filter can be ensured simply by reducing the interval $\bar{t}_f$ or using the algorithm II in the case of the ferrous form of contamination which is more economically efficient. It is necessary to take more serious measures with the oxide form of contamination, in particular, to use two-stage filters, etc.

It is easy to establish the optimal interval t_f, at which the reduced costs will be minimal when the filter is operated in accordance with the algorithm I and also the algorithms II, III possibly, if the dependence $RC(\bar{t}_f)$ is calculated. Fig. 12 shows three graphs of this dependence, which correspond to the basic values Ψ_0 and moderate contamination of the water supplied to the filter ($C_0 = 1\ mg/dm^3$). Therefore, it is obvious that the optimal relative value $\bar{t}_f$ is related to Ψ_0 respectively. Thus, it is enough to specify the function $RC(\bar{t}_f)$ in order to reduce the cost of the treated water to the minimum, using the algorithm I for a given initial ratio between the forms of iron. Approximate values of the desired optimums for $\bar{t}_f$ and RC correspond to the lowest point on this curve. Three values of t_f, corresponding to the condition $RC = \min$, namely $t_f = 800$, are obtained in this case at $\Psi_0 = 1$, $t_f = 700$, at $\Psi_0 = 0.5$, $t_f = 630$ and at $\Psi_0 = 0$. It is logical that the range of the practical values $\bar{t}_f$ decreases when C_0 increases and Ψ_0 decreases. Finally, this procedure of applied optimization of the technological process becomes impractical if $C_0 \geq 2.5 mg/dm^3$ and $\Psi_0 = 0$, since the filter cannot process such high levels of contamination.

The comprehensive view of the technological and economic indicators obtained as a result of purposeful long-term numerous calculations using the computer analysis resource (software package) Mathcad deserves a detailed discussion and comments. The complications that arose when calculating a large number of examples in relation to normal and extreme filtration conditions were mainly due to the choice of an overestimated duration of the operating interval $\bar{t}_f$ at the regular (first) filter operation algorithm. In this case, one of the ratios $t_f > t_h$ or $t_f > t_p$ took place in the worst case and the filter immediately turned out to be inefficient. The abrupt failure of the filter and the need for early replacement of the filter material as a result, was noted in a slightly better case but also undesirable for practical reasons. It was established that the algorithm I with an ultra-long interval $\bar{t}_f = 1200$ can only be used for very short operating intervals $\bar{t}_f$, and for the ferrous form of the initial water contamination. However, a significant reduction in the operating costs with such $\bar{t}_f$ does not significantly reduce the total costs. Moreover, there was even a noticeable increase in DC in comparison with the variant $\bar{t}_f = 900$.

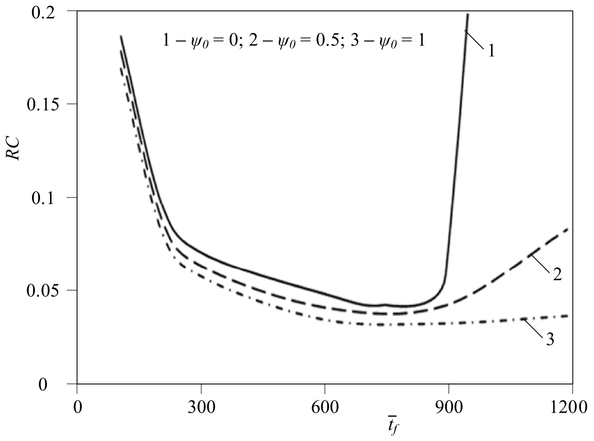

Fig. 12. Dependence $RC(\bar{t}_f)$, at $C_0 = 1\ mg/dm^3$.

It should be emphasized there is always a high probability the treatment treating resource of the filter will be insufficient in principle to solve the problem, based on the previous experience in a case of high levels of contamination of groundwater (it implies that the obtained filtrate will be high quality). Therefore, initially the filter cannot function in accordance with the established standards for the packed bed with the properties specified according to Ref. [19] when implementing the algorithm I, $\Psi_0 = 0$ (oxide form of contamination) and $C_0 \geq 2.5mg/dm^3$. There are different ways to resolve the situation in different ways. In particular, it is advisable to increase the height of the bed accordingly or reduce the (equivalent) size of its elements (grains) when the protective ability of the filter is low, especially if $\Psi_0 = 0 ... 0.5$. The next article from our series on physical and mathematical modeling of physical and chemical removal of iron from deep groundwater is planned to be dedicated to the rational choice of the main design factors.

Moreover, a significant initial content of ferric iron can also cause the practical unsuitability of the algorithms II, III. Indeed, at $C_0 \geq 2.5mg/dm^3$ in the absence of the adsorption process that prevents the transfer of iron ($C_{0a} = 0$), already due to the initial breakthrough of a great number of the oxide particles their concentration will immediately exceed the maximum allowable value C_*. In general, the expenses for iron removal when using the filter operation algorithms under consideration are comparable. However, a reasonable choice is important based on the specific filtration conditions of the operation algorithm and especially the operating interval in the case of the algorithm I. According to the obtained results of numerous technical and economic calculations with typical initial data, it can be concluded that the cost of clean water is 12% less in the case of the algorithm I, but only with a reasonable choice t_f (in the case under study, from 48 to 98 h with the optimal number of hours being 72) with a predominant content of ferrous iron in the groundwater and its relatively low contamination ($C_0 = 1 \ mg/dm^3$). A daily increase or decrease in t_f per day results in a 73% increase in *RC*.

Naturally the cost of water treatment becomes higher but noticeably faster with the implementation of the algorithm I when the level of the contamination increases and at the same standards of iron removal. Thus, pure water will be 16% cheaper even at $C_0 \geq 2.5mg/dm^3$ with the algorithm II. The cost of water treatment increases significantly with an increase in the proportion of oxide iron. The algorithm II allows to save 9 … 15%. Certainly, one should also keep in mind the additional difficulties with the control of the filtrate quality and head losses in the filter, which is necessary when operating according to the algorithm II and partially to the algorithm III in the final choice of the operation algorithm. The mathematical modeling methods can be of great help in a such situation.

Based on the date derived from numerous calculations, it is justified to conclude that the role of excessive oxygen concentration at iron removal from groundwater is negative from an economic point of view. The decrease in Ψ_0 first to 0.5 and then to 0 in all examples inevitably led to a noticeable increase in *RC* (from several percent to several tens of percent). At the same time, a decrease in Ψ_0 to 0 generally led to multiple increases in the cost of water treatment in certain situations, for example, in the case of the algorithm I and $C_0 = 2 \ mg/dm^3$. Particular attention should be paid to the cases of partial or complete incapacity of the filters when the initial content of ferric iron is high. If $\Psi_0 = 0$ then at $C_0 \geq 2.5mg/dm^3$ all three algorithms are unsuitable. Actually, it is not possible to achieve the required quality of the filtrate under the considered technological conditions, in principle, due to the rapid depletion of the adsorption capacity of the filter material. However, the situation changes drastically already at $\Psi_0 = 0.5$ and now the algorithm II makes it possible to remove iron from water at a moderate cost. The algorithm I provides the required quality and volume of pure water at an unnecessary higher cost, but only when $\bar{t}_f$ is selected correctly. If the values of $\bar{t}_f$ are too high, then the iron content in the filtrate can immediately exceed the values allowed by the standards.

4. Conclusions

1. It is advisable to conduct the optimization calculations during filtration at a constant rate taking into account the specifics of the physicochemical removal of iron from groundwater and using three criteria. They impose restrictions on the iron content in the filtrate (quality criterion), head losses in the deep bed (hydraulic criterion), deposit strength (consolidation criterion). The joint use of these criteria makes it possible to conduct technical and economic calculations taking into account not only the operating costs but also the capital costs. The developed calculation method allows to comprehensively determine the reduced costs for treating groundwater with excess content of iron, considering the service life of the bed and, accordingly, the cost of its replacement and the costs for regular backwashing of one medium change. As a result of systematic long-term calculations of examples with typical initial data, the patterns of changes in the capital, operating and reduced costs were established depending on the concentration and ratio of iron forms (ferrous/ferric) in the water in its initial state, three algorithms for controlling the operation of the filter.
2. The service life of the filter medium is an important indicator of the working ability of the filter-clarifiers. The specified period depends on the properties of the filter material, filtering conditions, filter control method, etc. The ratio of iron forms in the raw water significantly affects the efficiency of iron removal by filtration. It is possible to significantly increase the serviceability time for changing the material of the bed by reducing the content of ferric iron in the water in its initial state. The service life of the medium decreases as the initial iron concentration increases. It is possible to achieve longer service life of the bed with shorter filter runs using the regular filter control algorithm, that is a result of weaker deposit consolidation during every filter run. There is a maximum depletion of the treating resource throughout the entire sequence of filter runs, which contributes to the long-term operation of the filter material change when the irregular filter control algorithm is being used.
3. The service life of the medium is limited due to the rapid decrease in the capacity of the bed (hydraulic criterion) in the case of low concentrations of iron in the raw water. When the initial iron concentration increases, the specified period is already limited by the time of the protective action of the bed (first for ferric iron), regardless of the filter control algorithm.
4. Using the regular filter control algorithm, the operating costs are reduced with an increase in the duration of the filter run due to a decrease in the total number of backwashings per filtering material change. At the same time, the capital costs for replacing one bed

change increase, which is caused by its shorter service life. The clearly defined extremum is characteristic of the behavior of the marked indicators. For example, when $\Psi_0 = 1,0$, $C_0 = 1\ .5M\text{г}/\text{д}M^3$, then the lowest cost of the treated water is provided if the regular duration of the filter runs is 700 units (optimum).

5. As a result of a detailed analysis of the dependence of the reduced costs on the content and composition of contamination, the method of controlling the technological process, we conclude that the reduced costs with a decrease in the percentage of ferrous iron increase significantly in the case of the regular algorithm and a moderate iron content at the filter inlet. In general, the initial concentration of iron has a significant impact on the value of the reduced costs. The sensitivity of the reduced costs to the contamination composition parameter Ψ_0 increases multiple times with its increase. The reduced costs rise non-linearly as a level of contamination and the proportion of the ferric iron form in it increase. In this case, the efficiency of the filter is sharply reduced down to a critical level (the filter is initially unable to function; the regular duration of the filter run is less than the minimum allowable). In such situations, it is necessary to improve the design of the filter, apply multi-stage filtration, etc.

Author contribution statement

All authors listed have significantly contributed to the development and the writing of this article.

Data availability statement

Data included in article/supplementary material/referenced in article.

Additional information

No additional information is available for this paper.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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