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Modelling of iron concentration changes in tap water after sampling

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ABSTRACT

In most cases, it is impossible to analyse drinking water for iron content at the sampling point. The water needs to be transported to a specialized laboratory, which can take several hours. This also applies to tap water. It was previously established that iron in water quickly passes from soluble to insoluble form. As a result, its concentration within 90 minutes decreases by 1.5–2 times compared to the initial value. The aim of the research is to develop a new mathematical model for the prediction of the concentration of iron in drinking water depending on the duration of time from the moment of sampling to the moment of analysis. The model is based on empirical data obtained from measurements of iron concentration in tap water of the water supply system of the city of Pokrovsk, Donetsk region, Ukraine. Based on the analysis of four developed and analysed polynomial models for two samples of tap water, second-degree polynomial equations are recommended. A correlation analysis confirmed the presence a strong correlation of the iron content in tap water and the time interval between sampling and analysis. It was experimentally established that from the 90th minute the physical process of a parabolic decrease in the concentration of iron in tap water practically attenuate. The recommended time range for using proposed mathematical model is from 0 to 120 minutes from the moment of tap water sampling.

Keywords: tap water, iron concentration, mathematical model, spectrophotometric method, time

INTRODUCTION

Individual aspects of iron content in tap water are considered in different contexts. Previous studies of the behaviour of iron in water have found changes in its concentration in water over time. The first studies on changes in iron concentration in water over time involved studies of groundwater from flooded mines. These studies showed that iron concentration in water decreased exponentially over time, with a half-life of about 350 days [Frost, 1979]. According to some studies of surface waters in Northern Europe, changes in iron concentration in water over time may also be towards an increase in its concentration and can be caused by changes in redox conditions [Kritzberg and Ekström, 2012]. Such changes in the iron concentration in water, which are mainly caused by the dynamics of oxidation-reduction processes, are long-term in nature [Ekström et al., 2016]. Quantification of the presence and behaviour of dissolved Fe(II)/Fe(III), nano-particulate and micro-particulate iron in a net-acidic and net-alkaline coal mine drainages and passive treatment systems was carried out over a 12 month period [Matthies et al., 2012]. A study of the dynamics of the behaviour of dissolved iron over a 12-hour cycle showed its variable nature in various aquatic environments [Daneshvar, 2015]. During the study of changes in the chemical composition of water over time, dissolved iron was considered as one of the main factors in the multiple regression model [Dimberg and Bryhn, 2015].

Understanding the impact of different factors on the properties of the resulting iron particles is very important to improve the water quality in drinking water treatment and distribution systems. A study of water quality parameters, including pH, residual chlorine and others, shows their significant influence on the properties of iron particles and suspension in the drinking water distribution system. In drinking water treatment and distribution systems, soluble Fe(II) ions are oxidized to insoluble Fe(III) ions by the different variables and different reaction mechanisms that defines the chemistry of a typical drinking water distribution system [Rahman and Gagnon, 2014]. A study on the estimation and analysis of iron stability in drinking water distribution system was carried out in a city of China. It was found that iron ion was unstable, with a high $Fe(OH)_3$ precipitation tendency and obvious increase in turbidity [Niu et al., 2006]. There are studies that focus on modelling the distribution of iron concentration in water supply networks, including by geostatistical methods [Wojtkowska and Potyralla, 2022]. A mathematical model of the iron release flux in drinking water distribution system based on the pipe material, water chemistry and flow conditions was developed [Mutoti et al., 2007]. Mathematical models were developed to quantitatively reveal the relationship between iron release and the key quality parameters of iron pipes in water distribution systems. These models are applicable to predicting iron release during source water switch [Lin et al., 2021].

The modelling procedure can be successfully used to assess the long-term change in metal content in mine water, which is confirmed by practical results [Huisamen and Wolkersdorfer, 2016]. The concentration and ratios of iron forms in water in the initial state are used to model operating and capital costs in technical and economic calculations of the reduced costs for treating groundwater with excess content of iron [Poliakov and Martynov, 2023].

Water quality modelling in distribution networks has evolved to address challenges in predicting water quality changes from treatment plant to consumer. Possible applications of water quality modelling are considered in relation to water monitoring in water distribution systems [Woolschlager et al., 2005]. There are numerous mathematical models related to the solution of the problem of drinking water quality. Modelling tap water composition involves integrating various process models to predict water quality from source to consumer. A study of the dependence of the iron content in water supply networks on external factors showed that the iron concentration had a tendency to increase with an increase in the distance from the water treatment plant [Gražulevičienė and Balčius, 2009]. In addition to the hydraulic laws which describe the behaviour of water distribution systems behaviour, equations that describe the water quality in these systems are studied. These models are also focusing on simulation, optimization and water security modelling in water distribution systems [Ostfeld, 2005]. Modelling as a method for quantifying the reductive dissolution of iron oxides was used to investigate reductive iron-mineral transformations [Rawson et al., 2014]. To study the spatial and temporal patterns of drinking water parameters, a dynamic drinking water quality model was developed that linked physicochemical parameters to the water source and spatial and temporal variables. This model showed that sampling location and time are significant factors in changing physicochemical parameters, in particular iron content and turbidity [Tăban et al., 2023].

A linear regression model is proposed for estimating iron concentration in water, which is considered as an alternative to the colorimetric method. The advantage of using a linear regression model is that it eliminates the dependence on an expensive, non-portable, electric colorimeter, which includes manual pre-calibration with overhead costs for storing samples [Sayeed et al., 2020]. Regression analysis was used for a two-factor model of the dependence of iron concentration on tap water temperature for subsequent practical application [Di Caprio et al., 2024]. The importance of dispersion analysis in developing a probabilistic model of network water quality is emphasized. According to the authors, this approach is a new way to assess water quality in the drinking water distribution system [Blokker et al., 2008]. It is also proposed to use regression models as the simplest and fastest method of water quality monitoring to predict the concentration of anions, cations and heavy metals, thereby providing a realistic groundwater situation [Agori et al., 2021]. In addition to using the traditional mathematical models, the possibilities of using artificial intelligence to predict hydrological and chemical processes are being actively considered [Ramzi et al., 2024]. The use of artificial intelligence is proposed as a tool for predicting water quality and managing water resources [Zhu et al., 2022]. Artificial intelligence methods have demonstrated high performance in predicting water quality components [Haghiabi et al., 2018]. One successful example of the application of artificial intelligence is an artificial neural network model for predicting iron concentrations at wastewater treatment plants in Baghdad. The model was developed based on the assessment of water quality depending on iron concentrations at seven wastewater treatment plants [Al-Musawi, 2016].

As part of a study of tap water in Donetsk region, Ukraine, the process of stabilization of iron content in drinking water after sampling was investigated. It was found that the iron concentration in water after sampling spontaneously decreases, which is due to the course of oxidation and hydrolysis reactions [Zbykovskyy et al., 2024].

MATERIALS AND METHOD

Study area

Pokrovsk district is located in the southwestern part of Donetsk region in eastern Ukraine, covering a total area of 4004.1 km². The population of the district before war exceeded 400,000 people. This research was conducted in the city of Pokrovsk which is geographically located at coordinates 48°16’42.2”N 37°10’39.6”E. (Fig. 1). Nowadays, the city of Pokrovsk is in an active combat zone. The landscape of the Pokrovsk district is predominantly steppe, typical for eastern Ukraine. Due to the lack of atmospheric and groundwater, there are few rivers in Pokrovsk district. But these rivers are classified as small. Currently, a source of drinking water is used from the Karlivka Reservoir. And that is why the population of the region faces a catastrophic problem of shortage and quality of drinking water.

The composition of drinking water is extremely unstable, and the concentration of substances exceeds the maximum permissible standards. The main reason for this situation is the presence of a large number of industrial enterprises in the region, including those harmful and dangerous to the environment [Turchanina – Rybak et al., 2021]. The greatest danger is posed by coke-chemical plants [Starovoit et al., 2021; Pyshyev et al., 2023]. The biggest challenge is determining the true value of the iron content in water. This is due to the nature and characteristics of the behaviour of iron in aqueous solutions.

Materials

The object of the study was samples of drinking water from the centralized water supply systems of the city of Pokrovsk. The indicators that characterize the quality of tap water are as follows: total salt content is 397–586 ppm, total hardness is 7.2–8.8 mmol/litre, turbidity is 0.19–2.8 NTU, pH is 6.3–8.1.

Equipment

The spectrophotometer UNICO 2150UV (λ=200–1000 nm) was used as the main equipment for measuring the iron content in tap water samples (Fig. 2). For this experiment, 50 mm

Figure 1. Geographical location of drinking water sampling site

Figure 2. Spectrophotometer UNICO 2150UV for tap water analysis by photometry

thick glass cuvettes were also used. Using the UNICO 2150UV spectrophotometer for photometry involves measuring the intensity of light absorbed or transmitted by a sample at specific wavelengths, enabling precise quantitative and qualitative analyses. The wavelength range for determining iron content in water is within the working range of the spectrophotometer, which can operate in a wide wavelength range: from 200 nm to 1000 nm. Its versatility allows spectral analysis for the ultraviolet and visible wavelength ranges. The principle of this study is based on the construction of a calibration curve and the subsequent determination of the iron concentration in the water samples being studied.

Methodology of iron determination

To determine iron concentration, a calibration curve was constructed using the spectrophotometric method with 1,10-phenanthroline, which forms an orange-coloured complex with iron [Zbykovskyy et al., 2024]. Algorithm for determining the total iron content in water is shown in Figure 3. The idea of the experiment was to study changes in iron concentration in drinking water over time. It was suggested that there is a link between iron concentration in tap water and the length of time between sampling and analysis. This paper presents a new mathematical model for the prediction of the concentration of iron in drinking water depending on the duration of time from the moment of sampling to the moment of analysis. The model is designed on empirical data obtained during measurements of iron concentration in tap water from the water supply system of the city Pokrovsk, Donetsk region, Ukraine. This theoretical model is the basis for experiments aimed at determining the initial iron content in water when it is impossible to measure it directly at the sampling site.

RESULT AND DISCUSSION

Mathematical modelling

To develop a mathematical model of the behaviour of iron in water after sampling, a passive experiment was chosen, which is a traditional method for conducting a large series of experiments with variation of the influencing factor.

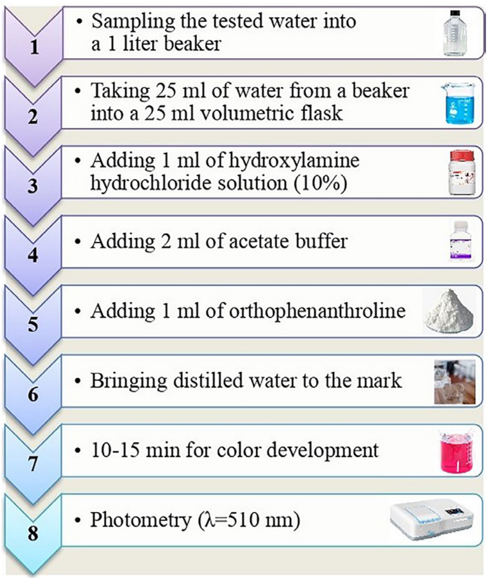

Figure 3. Algorithm for determining the total iron content in water

Processing of experimental data was carried out using statistical methods. Methods of mathematical statistics allow us to obtain a mathematical description of a process, which can be used in further research to predict the results of an experiment. The main advantage of these models is that they enable accurate forecasts when the initial conditions are known. However, the modelling results may be inaccurate outside the range of unambiguous conditions and are difficult to interpret.

The objective of the experiment was to develop an adequate mathematical model of changes in the concentration of iron in tap water depending on the time interval from the moment of sampling to the moment of analysis. This model can be used to determine the initial concentration of iron in tap water in situations where it is impossible to analyse water samples directly at the point of collection.

There are known studies on technological modelling of physical and chemical removal of iron from deep groundwater in Ukraine [Poliakov and Martynov, 2023]. As an input factor for constructing a mathematical model, the authors took water with an initial iron concentration of 1–3 mg/l. Taking into account the proven effect of reducing iron concentrations during the first two hours after sampling [Frost, 1979; Vijay et al., 2023], as well as the lack of information about the time and place of sampling, the proposed models are controversial.

Regression analysis is a versatile statistical tool that is commonly used to predict the values of a variable in chemical process studies [Alayat et al., 2018]. In this study, the regression equation is used to calculate the initial value of the required variable. This is fully consistent with the statement about the feasibility of using the correlation method to determine the concentration of a substance in chemical analyses and analytical measurements [Stalikas and Sakkas, 2024; Urban, 2020].

Research based on the reviewed articles shows that nonlinear polynomial models can be used to determine the concentration of iron and other substances [Faier Crivineanu et al., 2012; Abukhadra et al., 2015]. Similar studies demonstrate that nonlinear polynomial models can describe the processes of change in iron concentration in water with sufficiently high accuracy [Safonyk et al., 2019; Kvartenko and Prysiazhniuk, 2022]. To select a mathematical model, polynomial equations of the second, third, fourth and fifth degrees were determined. As a result of the calculations, equations of polynomial curves and determination coefficients for two samples of tap water were obtained. The samples had an iron concentration in water of 0.13 mg/l and 0.08 mg/l at the time of their collection from the water supply system (Table 1).

Comparison of the obtained polynomial equations showed that the values of the regression coefficients in the second-degree equations for both samples of tap water coincided. The values of the coefficients of determination for all four models are high: from 0.9473 for the second-degree equation to 1.000 for the fifth-degree equation. This fact confirms the high degree of reliability for the obtained mathematical equations in the specified area of study (the time interval after sampling from 0 to 150 minutes).

Mathematically, the obtained equations of the fifth degree are the most preferable, since the curves pass through all experimental points and the determination coefficient is equal to 1.000. Considering the possibilities of using polynomial models, the authors also point out the high

Table 1. Equations of polynomial curves and coefficients of determination for two samples of tap water

The type of mathematic model	Models of iron concentration changes in tap water over time	R^2
Model selection at the initial concentration of iron 0,13 mg/l		
Polynomial model of the second degree	$y = 4E\text{-}06x^2 - 0{,}0009x + 0{,}1258$	0,9473
Polynomial model of the third degree	$y = -4E\text{-}08x^3 + 1E\text{-}05x^2 - 0{,}0014x + 0{,}1293$	0,9927
Polynomial model of the fourth degree	$y = 4E\text{-}10x^4 - 2E\text{-}07x^3 + 3E\text{-}05x^2 - 0{,}0018x + 0{,}1299$	0,9974
Polynomial model of the fifth degree	$y = -1E\text{-}11x^5 + 5E\text{-}09x^4 - 8E\text{-}07x^3 + 6E\text{-}05x^2 - 0{,}0023x + 0{,}13$	1,0000
Model selection at the initial concentration of iron 0,08 mg/l		
Polynomial model of the second degree	$y = 4E\text{-}06x^2 - 0{,}0009x + 0{,}0773$	0,9756
Polynomial model of the third degree	$y = -3E\text{-}08x^3 + 1E\text{-}05x^2 - 0{,}0012x + 0{,}0795$	0,9935
Polynomial model of the fourth degree	$y = 2E\text{-}10x^4 - 9E\text{-}08x^3 + 2E\text{-}05x^2 - 0{,}0013x + 0{,}0798$	0,9946
Polynomial model of the fifth degree	$y = -2E\text{-}11x^5 + 7E\text{-}09x^4 - 1E\text{-}06x^3 + 6E\text{-}05x^2 - 0{,}0022x + 0{,}08$	1,0000

information accuracy of higher-degree models compared to second- and third-degree polynomial models [Rusu et al., 2018]. However, models of the third, fourth and fifth degrees have a significant weakness. It is that the change in the concentration of iron in tap water is a unidirectional physical process. At the same time, the curves, starting from the third degree, have a "wave-like" character, which has short-term intervals of increasing iron concentration with increasing time from the moment of water sampling (Fig. 4, 5).

Such behaviour of the curve does not correspond to the real physical process. In this case, equations of the third degree and higher are unacceptable for the physical interpretation of processes, since they simply adjust the calculated values to the empirical data. Therefore, these mathematical models cannot be used for extrapolation in solving such problems.

High degrees for mathematical models can be recommended for modelling processes with sudden changes, saturation or oscillations. In the process of decreasing the concentration of iron in water over time, such changes were not detected. At the same time, these models are cumbersome and difficult to calculate the initial concentration of the substance.

Second-degree equations are attractive not only because of the high value of the coefficient of determination, but also because of the

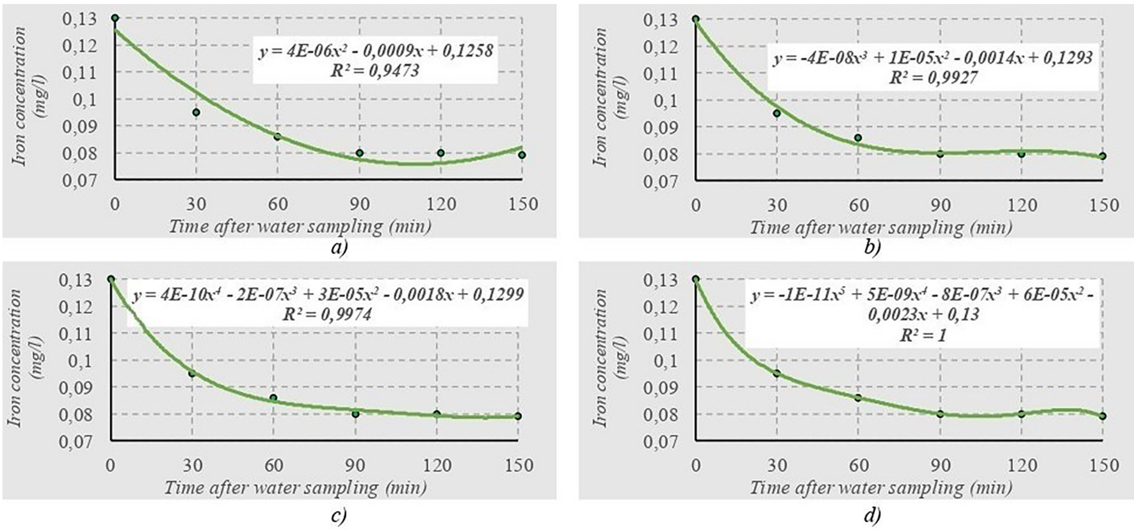

Figure 4. Mathematical models of iron concentration in tap water over time with an initial iron concentration 0,13 mg/l: (a) second degree; (b) third degree; (c) fourth degree; (d) fifth degree

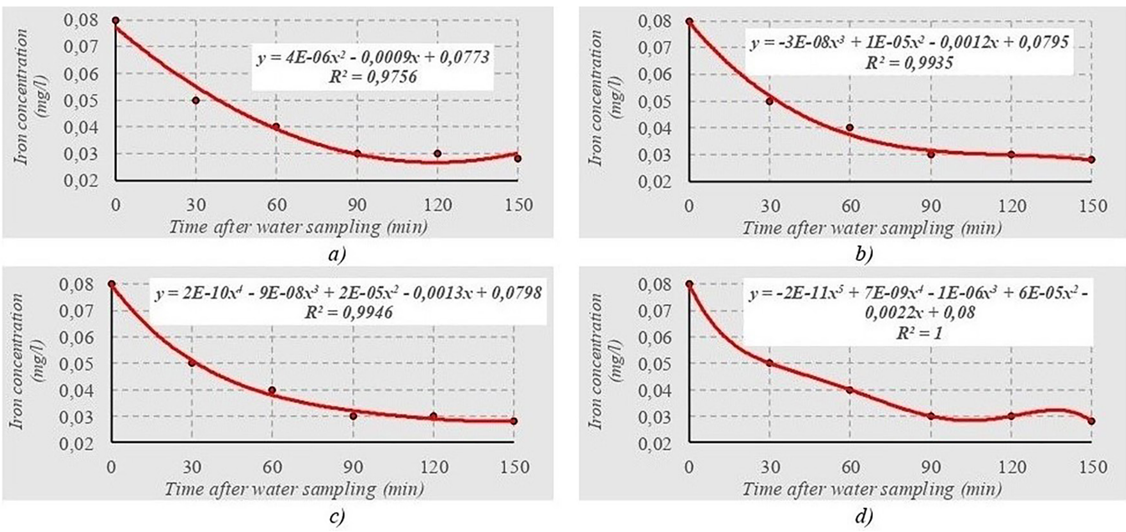

Figure 5. Mathematical models of iron concentration in tap water over time with an initial iron concentration 0,08 mg/l: (a) second degree; (b) third degree; (c) fourth degree; (d) fifth degree

simplicity of the model for practical application. The equality of the regression coefficients confirmed the identity of the physical process of changing the iron content in tap water in both samples. At the same time, it should be taken into account that the described physical process of parabolic decrease in iron concentration in tap water was recorded in a certain time interval from the moment of sampling. It was experimentally established that from the 90th minute the process of decreasing iron concentration practically attenuated. After 120 minutes, there was no change in iron concentration in water. Therefore, second-degree polynomial equations were chosen as a mathematical model (Table 2). The Eurachem Guide recommends that for each mathematical model obtained as a result of chemical analyses, it is mandatory to establish a «working range". Within this range, the resulting equation adequately describes the process with an acceptable level of uncertainty [Magnusson and Ornemark, 2014]. According to this statement, the recommended "working time range" for using these models for the variable x is from 0 to 120 minutes from the moment of sampling. The constant term of the regression equation represents the rate of change of y for small changes in x (the first derivative at the initial point). The second-degree coefficients describe nonlinear effects such as acceleration.

Additionally, the second-degree equations were tested for adequacy by calculating and comparing the calculated and empirical values of iron concentration in tap water for both samples. The statistical characteristics of the mathematical models for tap water samples 1 and 2 are given in Tables 3 and 4.

As a result, the recommended equation for determining the initial iron concentration in tap water will be as follows:

$$Y_0 = Y + 0{,}0009x - 4E\text{-}06x^2 \quad (1)$$

In this model, Y_0 is the initial concentration of iron in tap water, mg/l; Y is the concentration of iron in tap water after a time (x, min) - from the moment of sampling to the moment of analysis, mg/l.

The high value of the correlation coefficient R=0.9918 characterizes the presence of a very

Table 2. Mathematical models for determining the concentration of iron in tap water

Model selection	Models of iron concentration changes in tap water over time
The initial concentration of iron 0,13 mg/l	$y = 4E\text{-}06x^2 - 0{,}0009x + 0{,}1258$
The initial concentration of iron 0,08 mg/l	$y = 4E\text{-}06x^2 - 0{,}0009x + 0{,}0773$

Table 3. Statistical characteristics of the mathematical model for tap water sample 1

Time, min	Empirical value	Calculated value	Residual deviation	Relative deviation, %	Squared residual
0	0.130	0.1258	-0.0042	-3.23	0.00001760
30	0.095	0.1024	0.0074	7.78	0.00005480
60	0.086	0.0862	0.0002	0.23	0.00000004
90	0.080	0.0772	-0.0028	-3.50	0.00000884
120	0.080	0.0754	-0.0046	-5.75	0.00002120
150	0.079	0.0808	0.0018	2.27	0.00000324

Table 4. Statistical characteristics of the mathematical model for tap water sample 2

Time, min	Empirical value	Calculated value	Residual deviation	Relative deviation, %	Squared residual
0	0.080	0.0773	-0.0027	-3,38	0.00000729
30	0.050	0.0539	0.0039	7,80	0.00001521
60	0.040	0.0377	-0.0023	-5,75	0.00000529
90	0.030	0.0287	-0.0013	-4,33	0.00000169
120	0.030	0.0269	-0.0031	-10,33	0.00000961
150	0.028	0.0323	0.0043	15,36	0.00001849

strong connection between the value of iron concentration in tap water and the time interval from the moment of water sampling to the beginning of the analysis. The influence of the time factor x is predominant, 97.56% of the variation in y is associated with the influence of factor x. All other unaccounted factors, including random ones, have an extremely weak effect on the variation of the iron concentration in tap water. Their influence is 2.44%.

CONCLUSIONS

The goal of this paper is to justify the possibility of modelling the process of changing the concentration of iron in tap water over time. As a practical mathematical model, a polynomial function is proposed. Polynomial models of the second, third, fourth and fifth degrees were developed and analysed. Second-degree polynomial equations were chosen as mathematical models.

A correlation analysis between the iron content in tap water and the time interval between sampling and analysis was carried out for two samples with an initial iron concentration of 0.08 and 0.13 mg/l. A strong correlation was found for each equation. This underscores the influence of time factor on the iron content in tap water. The determination coefficient values were from 0.9473 to 1.0000. However, the curves, starting from the third degree, have a "wave-like" character, and do not reflect the essence of unidirectional physical and chemical processes in tap water over time.

It was experimentally established that from the 90th minute the process of decreasing iron concentration practically attenuated. Therefore, the recommended time range for using these models is from 0 to 120 minutes from the moment of sampling. Clearly, further empirical studies are needed to obtain further data on changes in iron concentrations in tap water beyond the recommended time range.

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