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## MATHEMATICAL MODELS AND ALGORITHMS FOR PREDICTING SURFACE WATER POLLUTION

**Abstract:** The article provides an approach to the development of algorithms for predicting the factors of contamination of substances, including radionuclides of surface waters in the area of operation of an industrial enterprise. The formalization of tasks and algorithms for predicting surface water pollution has been carried out. Simulations are performed with the Adaptive Neuro-Fuzzy Inference System in MATLAB using an Artificial Neural Network (ANN) and risk-based analysis using Monte Carlo Simulation (MCS).

**Key words:** pollutants, mathematical model, model calibration, rank correlation, Monte Carlo method, forecasting.

**Language:** English

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### Introduction

Mathematical models for water quality control can be effective tools for predicting and modeling the factors of pollutants, including radionuclides of surface waters in the area of operation of an industrial enterprise, to a certain extent, it saves labor and materials costs for a large number of chemical experiments. Depending on the desired conclusion, a

simple data-driven mathematical model or a very complex simulation model is used.

When considering the problems of modeling and monitoring the quality of surface waters, it is necessary to take into account both concentrated and dispersed sources of pollution. The potential for pollution from diffuse sources is greater, but the concentration of pollutants from them is usually lower

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than in wastewater from concentrated sources. The success of water protection from the effects of diffuse sources of pollution is determined by the application of the most effective measures for predicting the flow of pollutants in surface waters.

### RELATED WORK

Mathematical modeling involves the sequential execution of the following stages: building a mathematical model of the process under study, developing a calculation algorithm and a program for its implementation on a computer. Mathematical models of real investigated processes are complex and include systems of nonlinear functional differential equations. The study of mathematical models is carried out on the basis of methods of computational mathematics, which are based on difference methods for solving problems of mathematical physics. The modern stage of applied mathematics is characterized by the study of mathematical models with extensive use of computational tools [1, p.112].

The trend of mathematization of sciences, which has a long tradition, and the deep penetration of mathematical models into meaningful research allows us to consider the need for mathematics as the basis for the synthesis of various scientific directions [2].

A significant contribution to the development of this direction was made by the famous Russian mechanic NE Zhukovsky, in which he derived differential equations of motion and solved a number of specific problems of water inflow to wells [3].

### FORMULATION OF THE PROBLEM

Many procedures and considerations are made to run a complex model. Each step of the modeling process must be performed with precision and research.

Step 1: Plan the model study and select the appropriate model for the study.

This is necessary in order to determine the type of model that can be adapted to the current state of pollution of the water source. Different assessments are made for different concepts of water quality. Sometimes a water quality model is created using little or no data. In such cases, it is very difficult to decide which processes should be included in the model.

Step 2: Monitoring and data collection

It is important to know the prior data needed to calibrate the model and also to validate it to minimize error in the output. Regular data is collected from selected measuring sites for better forecasting and analysis of water quality.

Step 3: Setting up the model

During the stages of the modeling process, various refinements and observations are made to ensure the minimum error in the output of the model. At this stage, no further research on modeling approaches is carried out.

Step 4. Calibration and model verification

Known data is compared with unknown data during the calibration process. Calibration always contains found and remaining data after model calibration. The validation process ensures that the model is processed by the input data correctly and efficiently without significant biases.

Step 5: Evaluate Model Performance

Once the selected model has been calibrated and verified, it can be used for further analysis and comparison between different studies.

### SOLUTION OF THE TASK

Eleven physical and chemical parameters are selected for analysis: -indicator, sum of cations катионов ( $\text{Ca}^{3+}$ ,  $\text{Mg}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{NH}_4^+$ ) and sum of anions ( $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{Cl}^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ), total hardness and dry remainder.

Trend analysis determines whether measured values for a water quality parameter increase or decrease over a period that can be temporal or spatial. There are several statistical methods available for trend analysis depending on the characteristics of the water quality data. Spearman's rank correlation analysis was used for trend and correlation analysis.

Spearman's rank correlation coefficient ( $R_{sp}$ ) can be described as:

$$R_{sp} = 1 - \frac{11 \sum_{i=1}^n (D_i D_i)}{n(n^2 - 1)} \quad (1)$$

where  $n$  is the number of values in each water quality dataset,  $D$  - difference, and  $i$  - number in sequential order. The difference between the ratings can be calculated as:

$$D_i = K_{xi} - K_{yi} \quad (2)$$

where  $K_{xi}$  is the rating of the measured variable in sequential order;  $K_{yi}$  - the series of measurements is converted into its rank equivalents by assigning a sequential serial number to the measured variable in the original series;  $x$  to the corresponding ordinal in the ranked series  $y$ .

Spearman's rank correlation coefficient;  $R_{sp} = 0$ , under the null hypothesis  $H_0$  versus the alternative hypothesis under  $H_1$ ; there is a tendency when  $R_{sp} < 0$  or  $> 0$ . The above condition has been verified by test statistics.

$$t_t = R_{sp} \left[ \frac{n-2}{1-R_{sp}^2} \right]^{0.5} \quad (3)$$

where  $t_t$  is the Student's  $t$  distribution, with  $n-2$  degrees of freedom at a 5% significance level, the time series had no tendency if  $\{v, 2.5\} < t_t < \{v, 97.5\}$  Spearman's rank

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correlation and Student's t -distribution were estimated temporarily for each parameter of nine selected observational points from 2018 to 2020, so that find out the positive and negative tendencies of changes in surface water quality parameters in the area influenced by the industrial enterprise.

When calculating wastewater quality, the importance of different water quality parameters depends on the intended use of the water and in terms of its suitability for domestic purposes [4-7].

In the process of developing a mathematical model, the following steps were taken:

1. Water quality parameters of interest were identified and ranked according to acceptability for the intended use in the body of water.

2. The measured values of the parameters were calculated according to the developed equations for each parameter and compared with the curves of

subjective assessment, which consisted in the dimensionless value of the sub-index in the range from 0 to 1 for each parameter.

3. The algorithm for calculating and formulating the model was chosen taking into account the available data and assumptions.

A rating scale was prepared as shown in (Table 1) for a range of values for each parameter. The rating ranges from 0 to 100 and is divided into five intervals. A rating of  $X_r = 0$  means that the water quality parameter in the wastewater has the most desirable value. On the other hand,  $X_r = 100$  means that the parameter present in the water exceeds the standard maximum allowable limits and the water is highly contaminated. Other ratings fell between these two extremes and were  $X_r = 25$ ,  $X_r = 50$ ,  $X_r = 75$ ; which are intended for lightly polluted, moderately polluted and excessively polluted.

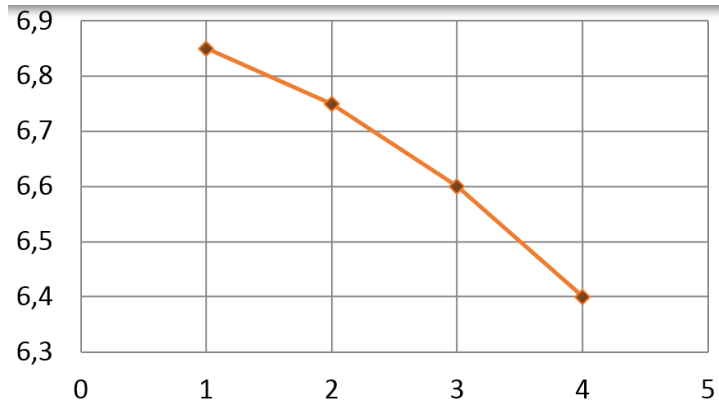
**Table 1. Rating scale for calculation**

| Water quality<br>Parameter                          | Ranges |                  |                    |                     |                    |
|---|--------|------------------|--------------------|---------------------|--------------------|
|   | pH     | 7,0-8,5          | 8,6-8,7<br>6,8-6,9 | 8,8-8,9<br>6,7-6,8  | 9,0-9,2<br>6.5-6.7 |
| Ca <sup>3+</sup> (мг/дм <sup>3</sup> )              | 30-140 | 140              | 150                | 160                 | 170                |
| Mg <sup>3+</sup> (мг/дм <sup>3</sup> )              | 20-85  | 85               | 90                 | 95                  | 100                |
| Fe <sup>3+</sup> (мг/дм <sup>3</sup> )              | 0,3    | 0,4              | 0,45               | 0,5                 | 0,55               |
| NH <sub>4</sub> <sup>+</sup> (мг/дм <sup>3</sup> )  | 0,5    | 0,6              | 0,65               | 0,7                 | 0,75               |
| CO <sub>3</sub> <sup>2-</sup> (мг/дм <sup>3</sup> ) | 0,5    | 0,6              | 0,65               | 0,7                 | 0,75               |
| HCO <sub>3</sub> <sup>-</sup> (мг/дм <sup>3</sup> ) | 0,5    | 0,6              | 0,65               | 0,7                 | 0,75               |
| SO <sub>4</sub> <sup>2-</sup> (мг/дм <sup>3</sup> ) | 500    | 525              | 550                | 600                 | 650                |
| Cl <sup>-</sup> (мг/дм <sup>3</sup> )               | 0,4    | 0,5              | 0,55               | 0,6                 | 0,65               |
| NO <sub>2</sub> <sup>-</sup> (мг/дм <sup>3</sup> )  | 3,0    | 3,5              | 4                  | 4,5                 | 5                  |
| NO <sub>3</sub> <sup>-</sup> (мг/дм <sup>3</sup> )  | 45     | 50               | 55                 | 60                  | 65                 |
| X <sub>r</sub>                                      | 0      | 25               | 50                 | 75                  | 100                |
| Pollution degree                                    | Clean  | Slight pollution | Moderate Pollution | Excessive pollution | Heavy pollution    |

The ranges of indicators of the quality of drinking water in accordance with the limits of its admission are shown in (figure - 1).

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**Figure 1 - Quarterly sampling time**

Building a mathematical model, you can see in the diagram how properties  $pH$  change when sampling from water on a quarterly basis.

Water quality ratings of  $pH$  require special handling and care. The permissible drinking water range  $pH$  is 7.0 to 8.5. A water quality rating of  $pH$  can be written as:

$$q_{pH} = 100[(v_{pH} - 7)/(8,5 - 7,0)] \quad (4)$$

where  $v_{pH}$  is the value  $pH \sim 7$ , which means the numerical difference between  $v_{pH}$  and 7.0 without regard to the algebraic sign. Equation (4) provides  $q_{pH} = 0$  for  $q_{pH} = 7.0$ . Quality ratings for other water quality parameters were calculated in the same way as water quality ratings for  $pH$ .

The more harmful this parameter of water quality, the lower its permissible value for drinking water. Thus, "weights" for parameters are different water quality parameters that are assumed to be inversely related to standards.

$$W_i = \frac{K}{S_i} \quad (5)$$

where  $W_i$  is the specific gravity for the  $i$ -th parameter of water quality ( $i = 1, 2, 3, \dots, 11$ ),  $K$  is a constant proportionality, which is determined from the condition and  $K = 1$  for simplicity. The values of  $k$  were calculated as:

$$k = \frac{1}{\sum_{i=1}^{11} (\frac{1}{x_i})} \quad (6)$$

Thus, the sum of the specific gravity 11 of the water quality parameter can be expressed as:

$$\sum_{i=1}^{11} W_i = 1 \quad (7)$$

All factors were weighted using the above equation.

Analysis of water quality in reservoirs is carried out using various methods, such as Spearman, rank correlation, calculation of parts of water quality parameters, multivariate analysis of variance with discriminant analysis, principal component analysis and factor analysis, canonical correlation analysis, cluster analysis. Simulations are performed using the Adaptive Neuro-Fuzzy Inference System in MATLAB, using an artificial neural network (ANN), and risk-based analysis using Monte Carlo Simulation (MCS). Error analysis and performance evaluations of these models were also performed to determine the most appropriate model for this study. [8-12].

## CONCLUSION

The findings from this research paper can be summarized as follows:

- From the calculation of the parts of the parameter in river water, it can be argued that the number of water parameters for three consecutive seasons follows the same trend. It can be concluded that the flow of wastewater into the river is constant throughout the year.
- To study spatial and temporal changes in water quality, multivariate statistical methods of discriminant analysis are used.
- Data on surface water quality for spatial changes and relationships between physical, chemical and biological parameters are assessed. Monitoring results have a greater impact on water quality main. The methods used here can offer an effective solution for water quality management in cases where quality data is complex.
- Correlation analysis shows that there is a moderate correlation between parameters due to land-use changes, mining operations and improper discharge of wastewater into the river. Therefore, it is vital to convert correlated parameters into uncorrelated parameters to effectively predict water quality.

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