Water Quality Assessment

Various human activities have been the main causes of surface water pollution. The uneven distribution of industrial enterprises in the territories of the main river basins of Ukraine do not always allow the real state of the water quality to be assessed.

1. Water Quality Assessment

Surface water quality monitoring is a complex procedure that includes a number of chemical analyses of water. In Ukraine, nine river basins have been identified, and water quality monitoring is carried out according to nine chemical indicators. The areas of river basins are quite significant and range from tens of thousands to hundreds of thousands of square kilometers [1]. The quality of surface waters is influenced by human activities. The activities of industrial enterprises, the mining industry and others always affect the environment to a certain extent. Thus, the qualitative and quantitative analysis of surface waters is directly dependent on anthropogenic impacts. For example, if there is a deposit of heavy metals in the area of a river basin and it is extracted, then such heavy metals should be included in the list of controlled chemical indicators [2]. If a chemical industry facility is located in the area of a river basin, the specific chemicals produced by that facility should be included.

Given the uneven distribution of industrial enterprises in the territories of the river basins in Ukraine, monitoring the quality of surface waters by nine indicators does not allow the real state of the water near the river to be assessed. When analyzing the above, it is expedient to select the necessary chemical indicators to monitor the quality of surface waters in accordance with a preliminary analysis of the anthropogenic impact on the basin of a particular river. Thus, it is advisable to make the list of controlled chemical indicators for water individually, depending on the type of anthropogenic activity [3][4]. The process of monitoring the quality of surface waters, including the systematic performance of chemical analyses of water, always comes with financial costs. If there are various industrial enterprises in the territory of a river basin, then the need to increase the number of controlled chemical indicators is obvious. In turn, this leads to an increase in monitoring costs. However, if there is no anthropogenic impact on the river basin, then the number of controlled chemical indicators of water quality can be reduced. This will reduce the cost of monitoring the water quality of such a river or an entire basin. It is important that with this approach, reducing the cost of monitoring such a river basin will increase the cost of monitoring a river basin with a high anthropogenic impact. There are various indices used to assess and monitor water quality in aquatic systems [5][6]. One of the first systems developed by Horton [7] was the creation of general indices that allow for the systematization of various water quality parameters. This methodology was then refined by the US National Sanitation Foundation (NSF), resulting in the well-known Water Quality Index (WQI) [8]. The WQI is an index that shows the level of cumulative influence of selected parameters on the overall water quality as a single numerical value [9][10]. This concept is widely used to assess water quality around the world [11][12].

A system for monitoring and assessing the quality of surface water, a method of examining individual sections of water in terms of their chemical, biological and nutritional components, has been introduced in many countries. Generic indices are used as comprehensive assessment tools that help assess water quality at an early stage and provide data and information for decision making by regulators. The assessment of water quality indicators makes it possible to establish the compliance or non-compliance of the water of a certain water body with requirements set by water users. The WQI has an advantage over other methods because it determines the overall water quality without interpreting individual factors [13]. Using a method that combines input parameters into a single resulting index has both advantages and limitations. The advantage is that the interpretation of the input variables is reduced to a single number, which makes it easier to understand the situation. The limitation of the method is due to the inability to assess individual factors, as well as the interdependence between them [14]. In addition, with numerous factors and data, calculating WQI can be time-

consuming and difficult. Therefore, various mathematical models, including fuzzy logic and ANNs, deserve consideration as alternative tools for the assessment of water quality [15].

2. Fuzzy Logic

The use of mathematical modeling allows situations that arise and proceed in an uncertain environment to be simulated. Given the dynamic variability and a significant number of variables, there is a trend in the mathematical modeling of water quality to develop methods that minimize uncertainty and facilitate the numerical solution of problems. One of the methods is fuzzy logic, which generalizes classical set theory and formal logic. Fuzzy logic is an extension of classical logic and can be used to solve problems that have a significant amount of subjectivity. The use of fuzzy logic was first proposed by the scientist Lotfi Zadeh in 1965 [16]. The main reason for the appearance of a new theory was the presence of fuzzy reasoning in the description of processes, systems and objects by a person.

Fuzzy logic is capable of handling linguistic, vague and uncertain data and can be defined as a logical, reliable and transparent process of collecting and using data that creates opportunities for decision making in the environment. The uniqueness of fuzzy logic is that it allows complex environmental problems with numerous input variables and complex interdependencies between them to be solved [17][18]. Fuzzy logic tools and capabilities are used to assess water quality by calculating the WQI [19]. Modeling ecological systems is a challenging scientific task because researchers often fail to make accurate statements about inputs and results. Fuzzy logic can be applied to the development of environmental monitoring indicators to solve this problem [20].

Due to its simplicity, fuzzy logic is successfully used to model natural-language-based water quality assessment [21]. Linguistic calculations used in fuzzy inference systems give better results than an algebraic expression for the estimation of the WQI. Fuzzy inference systems have been used to create water quality indices because these methods can provide alternative approximations when targets and boundaries are imprecise or poorly defined [22]. Thus, the authors conducted an extensive retrospective analysis of the evolution of methods for the calculation of the water quality index. Various options were analyzed, which concerned the choice of variables and the methods of weighting and aggregating these variables into a final value. The authors confirmed that the use of the fuzzy logic method can lead to significant progress in the methodology for the determination of the water quality index [23]. Caniani et al. [24] proposed to use a fuzzy model to assess the complex environmental vulnerability of an aquifer. The comparison of the obtained results with the traditional method showed that the fuzzy logic method turned out to be a useful and objective tool for environmental modeling. Yang et al. [25] created an early warning system aimed at accurately predicting algal blooms in rivers. The values of dissolved oxygen, velocity, ammonia nitrogen, total phosphorus and water temperature were used as input data for the fuzzy logic model. The fuzzy logic model successfully reproduced algal bloom events over a certain period of time. The authors of a study [26] used a Mamdani fuzzy logic model to classify groundwater quality for irrigation. The operation of the fuzzy model is based on the input membership functions of the electrical conductivity and sodium absorption coefficient, as well as on the output membership function of the irrigation water quality index.

Thus, the advantages of using fuzzy logic, compared to currently used water quality indices, are:

- The solution of issues with numerous input variables and complex interdependencies between them.

- The calculation of the final index occurs by evaluating the behavior of each analyzed parameter in relation to others.

3. Artificial Neural Network

A large amount of data have to be used to assess water quality. Traditional methods (for example, linear and non-linear regression) do not fully satisfy the needs of researchers, and artificial neural network (ANN) models come to the fore. ANNs are a family of models whose architecture is based on biological neural networks [27][28]. Scientists consider ANNs as a collection of artificial neurons that are systematized into one interconnected network. The neural network can detect implicit relationships between inputs and outputs and is able to predict the water quality index [29]. It is enough to train the network, and in the future, it will be able to predict values based on previous experience. In addition, ANN models are able to work effectively with a non-linear relationship between data and provide high accuracy of forecasts [30]. Creating an ANN requires an appropriate network structure, a number of inputs and outputs and the number of epochs used for simulation. The selection of the optimal network structure occurs by using experience and trial and error. Choosing the optimal network architecture, activation function, loss function and optimization algorithm is an important step to approximate complex non-linear relationships [31][32].

Modeling artificial neural networks for water quality prediction has been repeatedly used by scientists. Elkhatip and Komur [33] showed that the level of quality of forecasting by an ANN model has a strong dependence on the amount of initial data. Chen et al. [34] showed that ANN models demonstrate high potential for solving problems of the prediction of the quality of groundwater and surface water. Palani et al. [35] analyzed Multilayer Perceptron (MLP) and General Regression Neural Network (GRNN) models with various inputs chosen by incremental constructive methods for prediction. The authors proved that a small dataset was a significant disadvantage for creating an optimal neural network. Wang et al. used a three-level MLP framework with a Back-Propagation (BP) algorithm to predict Chl-a levels. The dataset was divided into training (75%) and test (25%) samples. The results showed that an ANN model can effectively predict the value of the resulting indicator [36]. Miao et al. [37] used the Back-Propagation Neural Network (BPNN) to predict COD and ammonia nitrogen levels. A random non-linear relationship between input and output data was identified using the sigmoid function. Singh et al. [38] used eleven variables for the output layer. The data were split into three parts: 60% training set, 20% validation set and 20% testing set. As a result of using the neural network, the predicted output values were close to the real data.

Chen et al. [39] scaled the datasets so that the values were between 0 and 1, which allowed the use of a sigmoid transfer function. They applied constructive and clipping stepwise methods to maximize model performance by constantly adjusting predictions. Markus et al. [40] used trial and error to create an ANN architecture in their study. The result showed that the use of an ANN can improve the accuracy of NO_3 prediction compared to previous studies. Al-Mahallawi [41] argued that ANNs can model the complex process of water quality assessment because they provide a relationship between non-linear input and output data. Ai and Kisi [42] tested various ANN models. The results of the comparison showed that the Rotated Binary Neural Network (RBNN) model performs better than MLP in predicting the level of dissolved oxygen. Baek et al. [43] used modular neural networks (MNNs) that could effectively solve the problem of not sufficiently accurate prediction. They used momentum gradient descent and the back-propagation of the Levenberg–Marquardt error (TRAINLM). Chen and Liu [44] used a sigmoid function in the hidden layer and a linear function in the output layer. As a result, it was proven that the Adaptive Neuro-Fuzzy Inference System (ANFIS) and BPNN can predict DO with high accuracy. Han et al. [45] used cross-correlation for BOD prediction and cross-information for DO to select input data. Ta and Wei [46] applied the Adam optimization method which could handle sparse gradients on noisy issues to train the Convolutional Neural Network (CNN) parameters.

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