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# *Artificial Neural Network Based Raman Spectroscopy System for Water Quality Monitoring*

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***Abstract:*** Raman spectroscopy has been widely used in the field of environmental protection. In order to accurately judge the scattering signal and spectrum of water pollutants, this paper uses the artificial neural network method to quickly identify the Raman spectrum of water pollutants, which provides a good scheme for rapid and intelligent identification of Raman spectrum. Through real-time monitoring of water pollution, not only the detection speed of water pollution is greatly improved, but also the rapid decision to prevent and control water pollution is made, It is of great significance to take corresponding measures. In this paper, a RS system for water quality monitoring (WQM) is designed based on ANN. It is verified that the system has high detection accuracy through pH detection of water quality, and the ANN model can accurately classify water quality categories.

## 1. Introduction

Water is the source of life. Since the reform and opening up, due to the rapid development of industry and people's weak awareness of environmental protection, water pollution has occurred from time to time, with factories discharging a lot of sewage, cyanobacteria outbreaks, domestic sewage flowing into rivers, and unfiltered drug use in aquaculture having a huge impact on the environment and people's normal production and life [1]. The scarcity of water resources per capita in China makes it all the more precious, so it is important to establish a water quality monitoring system.

Research into the water environment now focuses on wastewater monitoring, environmental monitoring, water quality prediction and emergency response systems. For example, some scholars have found that many existing WQM systems cannot be monitored for long periods of time, so they have built a WQM system on NB-IOT that solves the small monitoring and short monitoring problems in many systems [2]. Some scholars used high frequency samples from stable water sampling systems to improve the accuracy of water quality monitoring data, while being able to analyse water quality indicators using hydrological historical data change trend analysis graphs, and used big data communication networks to build a secure sensor network to achieve comprehensive monitoring of water quality information [3]. Some scholars have developed an independent water quality monitoring system using artificial intelligence technology. The intelligent computer to obtain water quality data, to achieve high quality monitoring of water quality indicators, the use of artificial intelligence to form a sensor network, and the use of nodes of the network energy detector to perform the monitoring of water quality, assessment of drinking water quality, specific parameters contain PH, turbidity, dissolved oxygen and temperature, etc., has great practical application value [4-5]. In order to achieve harmless water resources, we need to produce advanced water pollution control equipment and various WQM instruments as well as developing clean water production technologies.

This paper first introduces the concept and network model of ANN, and then analyzes the application of ANN in Raman spectrum processing. When building the WQM Raman spectrum system based on ANN, analyze the measurement methods of water temperature, pH, DO and other parameters, and propose the treatment process of ANN in pollutant Raman spectrum. Finally, this paper tests the accuracy of water quality pH value monitoring and water quality classification accuracy of the system to verify the feasibility of the system in WQM.

## 2. Basic Overview

### 2.1. Principle of Artificial Neural Network

(1) Human brain neuron

The human brain plays an important and integral role in the human organism, and intellectual activity and the development of the human mind cannot be directed without the brain. The nervous system is responsible for transmitting information to the human brain, but the nervous system is made up of tens of billions of neurons with a complex structure, which are organised and intertwined to form a vast network, and no machine technology is as complex as the structure of the human brain [6].

(2) Artificial Neural Network

Inspired by the nervous system of the human brain, researchers have developed artificial neural network (ANN) models that mimic intelligent behavioural processes. The main role of this imitative behaviour is that, on the one hand, artificial neural networks must also build on existing information training, i.e. training the network through instance learning; on the other hand, artificial neurons create memories in the network through changes in memory weights and quantify the results of data-specific learning [7-8].

ANNs can perform partitioned parallel processing of data and ANNs have the performance of problem optimisation decisions. It consists of simple neural processing units and has the advantage of highly parallel processing. Its network structure determines that it can not only preserve knowledge from experience, but can also always acquire knowledge from outside. When the model training is completed, the neural network model is able to quickly reflect the relationship between the output values of the functions of each network layer [9]. The neuron is the smallest unit of the ANN model and its learning process is the process of training the neuron with sample data to adjust the weight and limits [10]. the ANN's its mathematical model is shown in Figure 1.

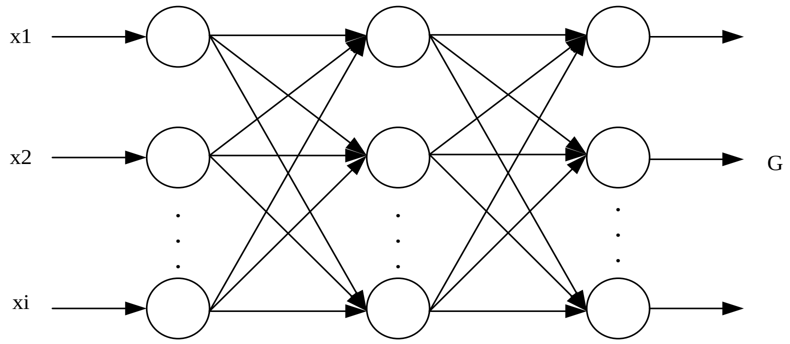


*Figure 1. Structure of neural network*

Assuming that the input signal of the sample data is X, the weight matrix is W, the threshold value is b, and F is the neuron activation function, the output response signal G is:

$$G = F(U + b) = F(W X^T + b) \tag{1}$$

where the weighted sum of the input signals U is :

$$U = \sum_{i=1}^{m} w_i x_i = W X^T \tag{2}$$

$$x_{k+1} = x_k - \alpha_k g_k \tag{3}$$

$x_k$ is the current network weight, $x_{k+1}$ is the later level network weight, $g_k$ is the gradient of the performance function and $\alpha_k$ is the learning rate.

The activation function F determines the value of the neuron output, removes redundant functions from some data, and has a great advantage in solving non-linear problems, enabling neuronal networks to solve complex problems better. The higher the function nonlinearity, the more features it can describe [11].

## 2.2. Artificial Neural Network for Raman Spectrum Processing

When light strikes matter, the light expands and other phenomena occur. Most of the light coincides with flexible matter with a constant frequency, which is partly known as Rayleigh scattering, while about a million beams of light collide with matter and the absorption or loss of energy causes an increase or decrease in wavelength, which is partly known as Raman scattering [12]. Depending on the frequency of the light, it can be divided into weak and strong light waves. Due to the weak scattering intensity, the Raman scattering intensity is only 10-6-10-7 times the incident light intensity, so its detection sensitivity is not suitable for the detection field compared to other spectra [13].

The spectral information interferes with the optical transmission and conversion of the photoelectric signal, thus affecting the useful spectral information of Raman. When a Raman spectrum is received, it must be converted [14]. The main ones are smoothing, compression and denoising.

(1) Compression of data

When a large amount of spectral data is available, the spectral function can be extracted for compression to remove it from the spectrum and improve data analysis, and it is particularly important to improve the retrieval performance of artificial neural networks for spectral data. This is particularly true for infrared spectra, many of which have covariance that is reduced even after compression [15-16]. Common compression methods include discrete wave compression, and discrete cosine transform. Discrete methods by cosine transform can avoid high infrared spectral dimensionality properties and have achieved good results in the reduction of spectral data dimensionality. Discrete wave compression is a very common mathematical transformation in recent years, and has good applications in spectral data compression [17].

(2) Smoothing of spectra

Smoothing refers to the averaging of data shifts. Smoothing methods such as window smoothing and median smoothing are used.

(3) Denoising of spectra

As Raman spectroscopy now mainly uses lasers as the excitation source, the laser intensity, background CCD conversion noise, current fluctuations and light propagation appear in a chain of noise that is inevitably generated during the spectrum acquisition process. The spectrum is denoised by methods such as Kalman filtering, median filtering [18]. Currently more commonly used is wavelet transform denoising.

## 3. Construction of WQM Raman Spectrum System Based on ANN

### 3.1. Collection of Water Quality Parameters

(1) Water temperature measurement

Currently, there are two main methods of monitoring water temperature, one is the method of detecting thermal resistance and the other is the method of detecting temperature differences. The method of detecting thermal resistance benefits from the high accuracy of measurement at low and medium temperatures, small fluctuations in measurement capacity and high stability. The temperature difference detection method uses the difference in electromagnetic forces to understand indirect temperature measurements, which can be obtained by the different electromagnetic properties of different materials at different temperatures. However, in general, the detection temperature difference due to the measurement of materials is more expensive, and temperature differences vary, not suitable for conventional water quality monitoring system, and the use of thermal resistance temperature sensor can be better adapted to water quality monitoring.

(2) pH measurement

PH value indicates the acid-base value of the solution, and the hydrogen ion concentration as a specific measurement of water quality can be measured by titration, electrochemical method, optical method, etc. In order to monitor water quality, pH sensors are usually processed on the electrochemical method, which is directly included in the power measurement. The potential difference between the two electrodes is due to the action of hydrogen, the magnitude of the potential difference is related to the concentration of hydrogen ions, PH measurement fluid can be achieved by processing the signal, perform unplanned automatic measurement.

(3) Dissolved oxygen measurement

Dissolved oxygen is a measure of the oxygen content of the solution, referred to as DO, dissolved oxygen in water measurement there are chemical, electrical and optical measurement methods, online measurement is mostly used when the electrical method and optical method. When measuring electrically, a voltage is applied to the cathode and anode, and the two poles and electrolyte form an electrolyte chain, resulting in an electrolyte reaction and current, which increases and decreases with the dissolved oxygen content in the water, therefore, the dissolved oxygen content can be obtained by measuring the electrolyte current value.

### 3.2. Raman Spectrum Data Processing Based on ANN

Raman spectroscopy data processing is an important component of a Raman spectrometer. A Raman spectroscopy software system can be understood as a collection of spectral identification, spectral noise filtering, spectral missing, spectral quality improvement, Raman spectral compatibility, spectral performance output, excess data elimination and spectral detection functions. The Raman contaminant index is high and manual identification is more difficult, whereas the use of a Raman spectroscopy system allows the spectrum to be detected by an artificial neural network algorithm. After the spectrometer has identified the relevant contaminant data, it has a clear understanding of the composition structure and other physicochemical properties of the contaminant and its toxicological data, based on the detection of the contaminant it can make emergency measures to deal with the damage to the environment caused by that contaminant.

After data pre-processing the corresponding spectra can be obtained. These spectra can better reflect the key properties of the material being measured. After receiving a spectrum of a substance, it is difficult to identify the spectrum manually and a suitable spectral signature needs to be found before a Raman panning operation can be performed. ANN is therefore used for Raman spectroscopy of water pollutants. The processing process of ANN-based Raman spectroscopy system for water quality monitoring is as follows: first filter the spectral data based on the pollutant sample library, extract the spectral data features through the artificial neural network, adjust the data into the network for spectral identification, then introduce the specific spectral data into the neuronal induction network, and get the standardised spectral data through the classification and identification of the spectra by the neural network the spectral data. The process is shown in Figure 2.

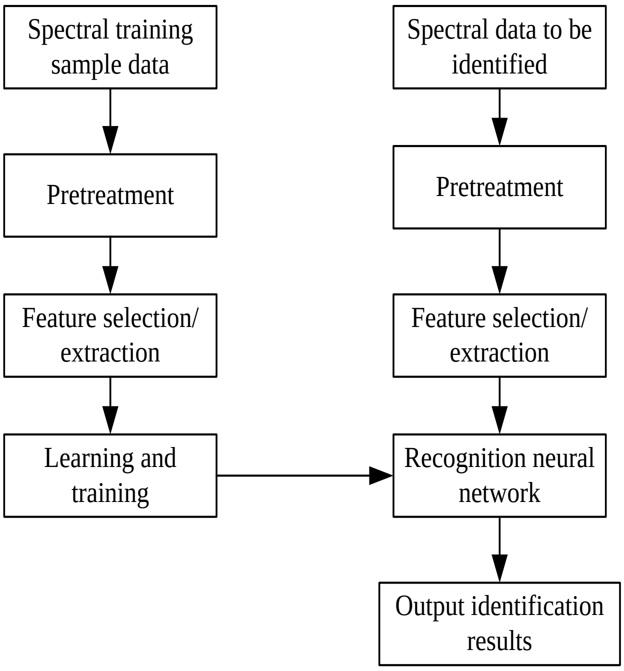


*Figure 2. Spectrum data processing flow*

## 4. WQM Raman Spectrum System Based on ANN

### 4.1. WQM Accuracy Test

As the accuracy of water quality monitoring is critical to respond to the actual water quality conditions, which also affects the accuracy of the system monitoring centre server, which sends commands to the system's terminals to collect information, so we must carry out accurate water quality monitoring tests. The experiment choose pH monitoring accuracy test as water quality monitoring accuracy test experiment, give the water quality monitoring accuracy test experiment scheme is the system water quality pH detection accuracy and manual water quality pH detection accuracy for comparison. Water quality monitoring accuracy test experiment specific process is as follows.

The first step is to obtain information about the system and establish a computer environment for the experiment based on the data collection and connection equipment requirements of the terminal design. In the second step, the programmed data collection program includes the micro-control used to control the water quality sensor. In the third step, the water quality sensors are set up according to the schedule and the micro-controller controls the pH sensors by starting the data collection program in order to collect pH data while performing manual detection and testing. In order to avoid the test experiment results with chance, here a total of eight sets of test experiments are conducted, and finally the eight sets of experimental results of the two testing methods are compared. The results of the system monitoring accuracy and manual monitoring accuracy are shown in Table 1 and Figure 3.

*Table 1. pH value of WQM*

| | System detection | Manual detection | Detection accuracy |
|---|---|---|---|
| 1 | 9.4 | 9.3 | 99.2% |
| 2 | 9.5 | 9.2 | 99.3% |
| 3 | 9.6 | 9.3 | 99.6% |
| 4 | 9.5 | 9.2 | 100% |
| 5 | 9.3 | 9.3 | 98.7% |
| 6 | 9.7 | 9.6 | 99.5% |
| 7 | 9.6 | 9.3 | 100% |
| 8 | 9.4 | 9.4 | 98.9% |

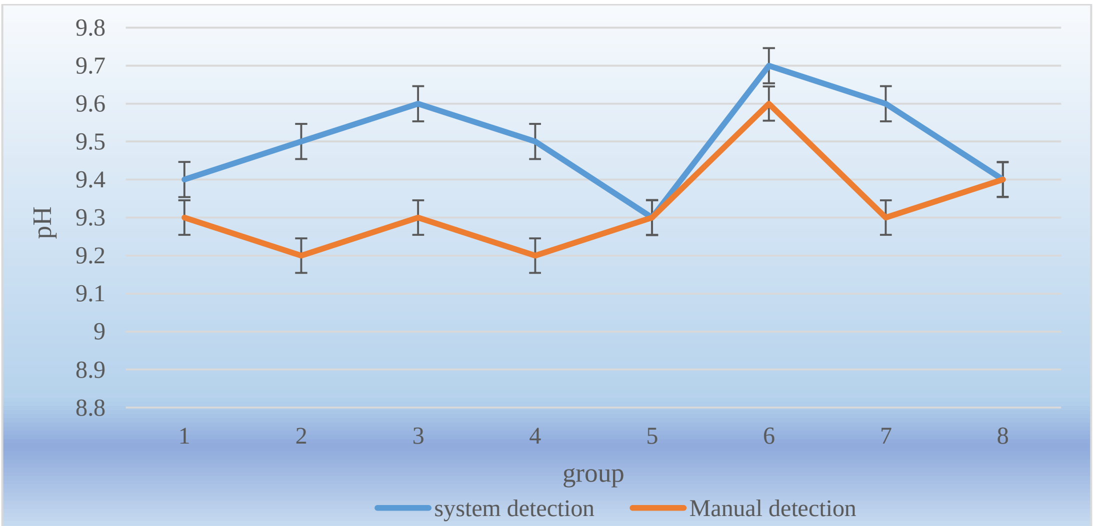


*Figure 3. Comparison between manual detection and system monitoring*

In Table 1, the maximum deviation between the measured data of pH sensor and the results of manual detection is 0.3, and the detection accuracy is above 98.5%. The detection accuracy of this system is very high.

### 4.2. Pollutant Classification Accuracy Based on ANN and Raman Spectroscopy


*Figure 4. Water quality classification accuracy*

The ANN and Raman spectra are applied to the detection of water pollutants, and the classification accuracy of different water quality categories is obtained through the identification of pollutant spectra by the ANN model, as shown in Figure 4. It can be seen from the table that the application of the WQM Raman spectroscopy system based on ANN to water quality classification is highly feasible, which can better provide a reliable basis for sewage monitoring and treatment.

## 5. Conclusion

Water is an indispensable and important resource in human production activities and social development. However, in recent years, the problem of water pollution has become increasingly prominent, and WQM has become a key issue in the protection and utilization of water resources. Therefore, this paper studies a WQM system that is easy to build and has timely and efficient monitoring results. At the same time, in order to manage, count and analyze a large number of water quality parameter data received by the monitoring system, this paper uses the Raman spectroscopy system to process the water quality parameter data, and combines the ANN model to identify water pollutants, thus realizing the high efficiency of sewage monitoring and treatment.

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## Data Availability

Data sharing is not applicable to this article as no new data were created or analysed in this study.

## Conflict of Interest

The author states that this article has no conflict of interest.

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