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Research and application of near-infrared spectroscopy in rapid detection of water pollution

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ABSTRACT

Objective: To study the method of rapid detection of water quality by means of near-infrared spectroscopy. *Methods*: Adopting USB2000 fiber optic spectrometer to carry out the near-infrared spectra for different water collected in the natural environment, comparing the reflectance rate between the polluted lake water and clean lake water in different regions, and making comparison on the reflectance rate of clean water in different water environment, so as to learn the changes of the near-infrared spectroscopy. *Results*: There are different absorption peaks and peaks in polluted and non-polluted water, and the trend of the reflectance spectra for water in different environments is approximately the same. *Conclusion*: Spectra technology has the advantages of low cost and easy operation and so on, which reflects its advantages in water quality detection. It has a good effect on solving water pollution problem, which has great significance for water quality monitoring.

Keywords: Water pollution; Near-infrared spectroscopy; Rapid test

1. Introduction

Water pollution has become one of the most important restrictive factors for the economic and social development of our country, which has aroused great attention of the government as well as the local government [1]. Our country has carried out a series of measures in science and technology, education, policy and so on, which has played an important role in curbing the deterioration of water environment [2]. In order to solve the existing water pollution problems, it is necessary to rely on the support of science and technology, also it is necessary that governments and enterprises at all levels continue to increase water pollution control and control infrastructure investment. At present, the most commonly used and effective method for water quality detection in China is spectrum technology [3].

In organic molecules, atoms with chemical bonds or functional groups are in constant vibration state, and their vibration frequencies are equivalent to the vibration frequencies of the near-infrared light [4]. Therefore, when we use near-infrared light to irradiate the organic molecules, the molecules in chemical bond or the functional group can vary on vibration and absorption, since the different chemical bonds or functional groups have different absorption frequency, therefore they exist in different position in near-infrared spectrum, so as to contain the information that the chemical bonds or functional groups obtained in the molecule. If we want to control the water pollution problem, it is the premise to distinguish whether the water is polluted or not.

The study on spectral reflectance of contaminated water can analyze, what is the difference between reflectance rate of the polluted water and clean water, as well as the difference between water reflectance rate in different regions, so that the relevant departments can find out the contaminated water more effectively, so as to use different standards to detect water pollution more effectively based on different regions [5]. At present, China's water environment quality monitoring technology has been developing rapidly, the current water quality monitoring technology in China is mainly by physical and chemical monitoring technique, including chemical method, electrochemical method,

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atomic absorption spectrophotometer, ion selective electrode method, ion chromatography, gas chromatography, plasma emission spectroscopy (ICP-AES) method and so on. Among these methods, spectral spectroscopy is the most widely used method in China. Spectrum technology has many advantages, such as wide monitoring range, high speed, low cost and long-term dynamic monitoring, so it has been applied to water quality detection in many countries. By now, near-infrared spectroscopy technology has got a lot of applications in water quality detection, China has taken the total nitrogen content and total phosphorus content as important indicators of water quality testing. In addition, we can measure COD, pH, heavy metal content and so on. The application of near-infrared spectroscopy technology has penetrated into all walks of life, including: petroleum and petrochemical, basic organic chemistry, fine chemicals, metallurgy, life sciences, pharmaceuticals, agriculture, food, paper making and so on [6]. It can also be widely used in celestial research, metal detection, rare elements and radioactive element detection, and many other aspects [7].

In this paper, through analyzing the near-infrared spectroscopy in different water, so as to study the rapid detection of water pollution, we can explore new method for detecting water pollution easily and rapidly at low cost.

2. Experiment and method

USB2000 optical fiber spectrometer is used in this experiment, the spectral range is between 390 to 1,000 nm and the resolution rate is 1.5 nm [8]. The natural light sources of surface water mainly include sunlight, moonlight and artificial lights and so on. The experiment uses tungsten lamp as the illumination condition to measure.

The location to intake the experimental water is Erlongshan reservoir in Laoshan, Qingdao (hereinafter referred to as A Lake), and the small West Lake in Zhongshan Park (hereinafter referred to as B Lake).

This experiment is mainly based on the comparison of the reflectance rate of the polluted lake water and clean lake water, the comparison of reflectance rate of clean lake water in different areas, and the comparison of reflectance rate of the same water in different environments [9]. In this experiment, two cups of clean water from Lake A and Lake B are chosen. And from the bottom of the water to collect the amount of sediment into three cups of water, standing for 15 h. Put the preparation of sewage from Lake A into one of two cups, standing for a while, so as to make full contact with water into a stable emulsion. Taking it as the polluted lake water [10], connect the computer with USB2000 fiber optic spectrometer, remove tungsten lamp and power source, then the light can be projected onto the board for the purpose of experiment, probe alignment point on the board, opening the spectra suite software, take the measured spectrum of light source as a reference spectrum and then saved, then the tungsten lamp can be closed, with a black board blocking probe, the spectrum results can be saved as the dark spectrum. Place the polluted lake water in the container to the point that is measured by the probe, so as to measure and preserve the spectral data. Under the same condition, the reflectance spectrum of clean lake water is measured and the spectral data can be preserved. The two groups of experimental data can be compared. Select the clean lake water from different areas, and the reflectance spectrum can be detected under the irradiation of tungsten lamp, then the data can be preserved and compared. Connect the computer with USB2000 fiber spectrometer, the sun light is projected onto the board for the purpose of experiment, probe alignment point on the board, opening the SpectraSuite software, take the measured spectrum of light source as a reference spectrum and then saved, then the tungsten lamp can be closed, with a black board blocking probe, the resulting spectrum can be saved as the dark spectrum. The probe is aligned with the outside lake water to measure and preserve spectral data. In the room, replace the sun with a tungsten lamp, then carry on experiment again.

3. Result and discussion

3.1. Test result

The experimental result can be shown in Fig. 1. Comparing and making contrast on these two sets of data measured under the tungsten lamp. It is found that both of them have a small absorption peak at 440 and 760 nm, and there is a peak at 710 and 810 nm. The polluted lake water tends to be stable in the 450 to 600 nm band. After 600 nm, with the increase of the wavelength, the reflectance rate decreases inversely, from 450 to 850 nm, the reflectance rate is over 20%. The reflection spectrum of clean lake water is relatively stable and the reflectance rate is below 20% (Fig. 2). Comparing these two sets of data measured under the tungsten lamp, we can see that the reflectance spectrum of lake water in different areas is approximately the same, and the reflectance rate of Lake B is slightly higher than that of Lake A. There are peaks in 420, 710 and 820 nm; Lake B has absorption peak at 770 nm; Lake A has absorption peak at 680 nm. The reflectance rate of these

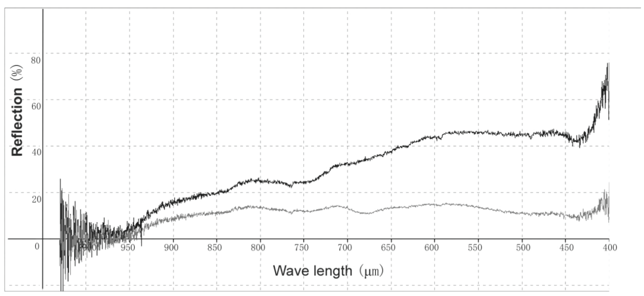

Fig. 1. Reflectance spectrums comparison between contaminated lake and clean water.

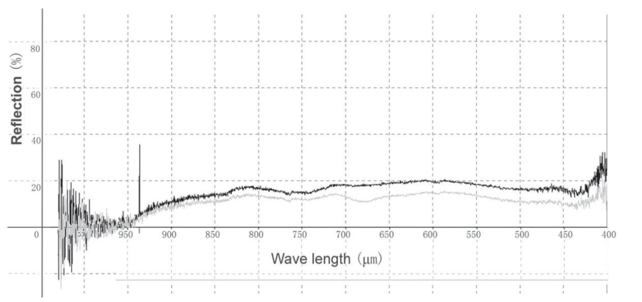

Fig. 2. Reflectance spectrums comparison between Lake A and Lake B.

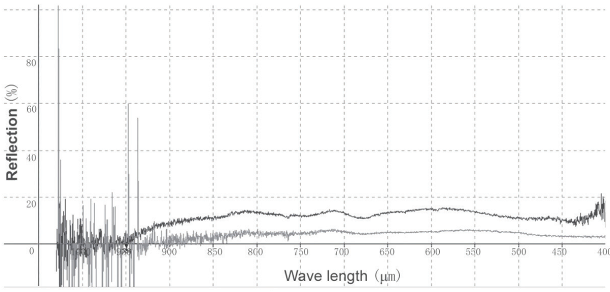

Fig. 3. Comparison of reflectance spectrums for same water body in different environments.

Table 1
Species and main sources of organic matter in water

Organic pollutant species	Main source
Halogenated hydrocarbon	By-product of chemical industry, organic solvent in metal cleaning, degreasing process, etc.
Benzene series pollutants	Industrial wastewater discharge
Chlorobenzene	Crop insecticide
Polycyclic aromatic hydrocarbons	Forest fire produced and infiltrated into groundwater
Chlorophenols	Widely used in wood preservatives, herbicides and pesticides
Organic pesticide pollutant	Heavy use of fertilizers, pesticides and herbicides in agricultural production

two clean lake water is below 20% (Fig. 3). It is found that the reflectance rate of the outdoor lake water is lower than that of the indoor lake water, and the reflection spectrum is more gentle; the indoor water has absorption peak at 670 and 750 nm. The reflectance spectra of the same water in different environments are approximately the same.

After the experiment, the polluted lake water was analyzed by infrared spectrum. The main pollutants and sources in the water are shown in Table 1. Due to the limitations of near infrared spectroscopy, only the species of pollutants can be resolved, and their concentration can be compared simply according to the height of the peak, but it cannot be quantified accurately.

3.2. Experimental error analysis

In the experiment, the micro-optical fiber spectrometer is used to measure indoor, which can exclude the influence of light intensity change, but not the humidity and temperature change. Because there is no corresponding supporting rod, the change of the angle and height of the detector becomes the biggest interference to obtain accurate data. As far as possible, one person can hold the detector without changing the height and direction, pointing to a certain point, only moving the experimental vessel, which can reduce the error effectively. In the outdoors, the water reflected spectrum will be affected by the weather, which may affect the reflection spectrum of sunlight.

4. Discussion

Through the experiment, we know that under the condition of the tungsten lamp, at 440 and 760 nm, there is a small absorption peak for both the contaminated water and clean water, at 710 and 820 nm, it can get its climax peak; Although there exists a difference between Lake A and Lake B, the overall trend is the same, the peak occurs at 460, 710, and 820 nm, there is an absorption peak at 840 and 760 nm, while Lake A has an absorption peak at 680 nm.

Through the experiment we know that the clear lake water in different areas may make the reflectance spectrum of lake water slightly different, while the trend of clean lake water spectrum remains unchanged.

The experimental results show that the polluted lake water tends to be stable at 450 to 600 nm. After 600 nm, with the increase of the wavelength, the reflectance rate decreases inversely, from 450 to 850 nm, the reflectance rate is over 20%. The reflection spectrum of clean lake water is relatively stable and the reflectance rate is below 20%. Thus, the reflectance spectrum of lake water in different areas is approximately the same, and the reflectance rate of Lake B is slightly higher than that of Lake A. There are peaks in 420, 710 and 820 nm; Lake B has absorption peak at 770 nm; Lake A has absorption peak at 680 nm. The reflectance rate of these two clean lake water is below 20%.

In the experiment of measuring the different environments of the same water body, the overall trend of these two is approximately the same. The different environments have little influence on the reflectance spectrum of water.

5. Conclusion

Through the research on the visible light spectral reflectance mapping experiment, the water pollution will have an impact on water reflectance rate. According to Fig. 3, the reflectance rate of the polluted lake water is relatively stable from 400 to 600 nm, and the reflection spectrum is little affected by the wavelength. Thus the peak value of water lake reflectance and trend can be used to distinguish whether there is water pollution or not; while water lake reflectance rate in different regions may be different due to environmental factors, aquatic organisms and other issues, but the overall trend is consistent, and the reflectance peak can be below 20%. Therefore, water from different regions has little influence on the reflectance spectrum.

Through the research on reflectance spectrum in near-infrared band, it is of great help to the detection of water pollution and the distinction of water pollution by using spectral characteristics.

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