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Non-Contact Measurement of Alcohol Content Based on Near Infrared Spectroscopy

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ABSTRACT

In order to solve the influence of other external factors on the measurement concentration of alcohol solution, a non-contact measurement method based on near-infrared spectroscopy and BP neural network temperature correction method was proposed in this paper. This method takes into account the influence of temperature on the light intensity of alcohol liquid solution in the detection process, and trains it together with the measurement data as the input of neural network. At the same time, it is compared with the index fitting algorithm, which proves that the method has a good effect on the non-contact measurement of alcohol content.

KEYWORDS

Near Infrared Spectrum; Alcoholic Strength; BP Neural Network; Intelligent Detection

1. INTRODUCTION

With the development of society and the improvement of people's living standards, the detection of alcohol has been paid more and more attention. The traditional method of alcohol detection usually requires contact with the tested sample, which has certain limitations. Non-contact measurement system, as a new detection technology, has the advantages of simple operation, fast and accurate, and has been widely concerned[1]. At present, the research on non-contact measuring system of alcohol has made some progress[2]. Many scholars and institutions are committed to developing a variety of non-contact measurement systems based on infrared spectroscopy, laser technology, image processing and other principles for alcohol detection and monitoring[3]. These systems have achieved some success in laboratory and practical application, providing a new idea and method for alcohol detection.

2. ANALYSIS AND SELECTION OF DETECTION SCHEME

2.1. Electrochemical Sensor Method

Electrochemical Sensor Method is a common method of alcohol detection, mainly for rapid determination of alcohol concentration, for example in drunk driving tests[4-5]. The working principle of this method is based on the oxidation of alcohol under certain conditions to produce an electric current. The electrochemical alcohol sensor is mainly composed of two parts: electrode and electrolyte. The electrodes are usually made of platinum and silver, and the electrolyte is a solution containing sulfuric acid. When the alcohol vapor enters the sensor, an oxidation reaction occurs on the electrode:

$$C_2H_5OH+H_2O \rightarrow CH_3COOH+4H^{+}+4e^{-} \quad (1)$$

This reaction produces electrons, which creates an electric current. The size of the current is proportional to the concentration of alcohol, so the amount of alcohol can be determined by measuring the current or voltage change in the electrochemical reaction. Electrochemical alcohol sensors are often used to make portable alcohol detectors, such as alcohol breath testers. When in use, the user only needs to blow on the instrument, and the instrument can measure the concentration of alcohol. The measurement results are usually available in a few seconds, which is very fast and convenient.

2.2. Near-Infrared Spectroscopy

Near-Infrared Spectroscopy is a non-destructive, rapid analysis method, widely used in food, chemical, medicine and other fields. For the detection of alcohol, near infrared spectroscopy is also a very effective method[6]. The basic principle is to irradiate the sample with near-infrared light (wavelength between about 780-2500 nm), and then measure the absorption and scattering of the sample to the near-infrared light. Different substances have different absorption and scattering properties for near-infrared light, so the composition and concentration of the sample can be determined by analyzing the near-infrared spectrum.

In the detection of alcohol, alcohol (mainly ethanol) has specific absorption characteristics in the near infrared region, and the alcohol content can be calculated by measuring the absorption of the sample to the specific wavelength of near-infrared light, so the concentration of alcohol can be determined by measuring the near-infrared spectrum.

The use of near-infrared spectroscopy for alcohol detection usually requires the following steps:

Sample preparation: Obtain the sample to be tested for sample preparation, if it is a solid sample, it needs to be pre-treated;

Spectral measurement: The sample is placed on the sample table of the NIR spectrometer, and the spectral measurement is performed[7]. During the measurement, near-infrared light is illuminated onto the sample, and then the sample's absorption and scattering of near-infrared light is measured.

Data analysis: Special spectral analysis software is used to analyze the measured spectral data, extract the absorption characteristics of alcohol, and then calculate the concentration of alcohol through the pre-established calibration model.

2.3. Photoelectronic Nose Method

Photoelectronic Nose Method is a sensor system that simulates human sense of smell. The basic principle of photoelectronic nose method is to identify and quantify the composition of gas by detecting and analyzing the optical properties of gas by using photosensitive materials with specific spectral response characteristics[8]. In the detection of alcohol, the optical electronic nose can determine the concentration of alcohol by detecting the absorption or scattering of light from alcohol vapor.

A photoelectronic nose usually consists of a light source, a gas absorption cavity, and a photodetector. The working principle is to use the light source to emit a specific wavelength of light, light through the gas absorption cavity to the gas sample, and then by the light detector to detect the light intensity after passing the gas absorption cavity[9]. Different gases have different absorption properties for different wavelengths of light. Therefore, by measuring the absorption of different wavelengths of light, the spectrum of the gas can be obtained, thus identifying and quantifying the composition of the gas. In the detection of alcohol, alcohol (mainly ethanol) has specific absorption characteristics for specific wavelengths of light, and the concentration of alcohol can be determined by measuring the spectrum of alcohol vapor.

The following steps are usually required when using the optical electronic nose method for alcohol detection:

Sample preparation: The first step is to obtain the sample to be tested. For liquid samples (such as alcoholic beverages), it is necessary to evaporate them into a gas; For solid samples, such as solid alcohol, pre-treatment may be required.

Spectral measurement: The gas sample is introduced into the gas absorption chamber and then the spectral measurement is performed[10]. In the measurement process, the light source emits a specific wavelength of light, which is irradiated to the gas sample through the gas absorption cavity, and then the light intensity after passing the gas absorption cavity is detected by the photodetector. Finally, special software is used to analyze the spectral data obtained from the measurement, extract the absorption characteristics of alcohol, and then calculate the alcohol concentration through the pre-established calibration model.

The advantages and disadvantages of the three methods are shown in Table 1-1.

Table 1-1 Analysis and comparison table

Method	Electrochemical Method	Near-Infrared Spectroscopy	Photoelectronic Nose Method
Advantage	Fast reaction speed, high sensitivity, continuous measurement, small and easy to carry, no need for external power supply	Non-destructive, fast and non-destructive, no sample pretreatment, real-time online detection can be achieved, and the cost is relatively low	Non-destructive, fast, simultaneous multi-component measurement, on-line detection, not susceptible to electromagnetic interference, good stability
Shortcoming	Easy to be disturbed by other volatile substances, short service life, easy to be disturbed by the environment, need multiple calibration, cumbersome operation	A large amount of experimental data and experience are required, and the price of spectrometer equipment is relatively high	It requires a large amount of experimental data and experience, low concentration substances are difficult to analyze, equipment is expensive and high requirements for operators

The advantages and disadvantages of the above three schemes are analyzed and compared. The detection scheme based on near infrared spectroscopy has high detection accuracy, relatively low cost, online non-destructive testing and wide application range. Although the detection accuracy will be affected by temperature, this defect can be remedied by temperature compensation and temperature correction. Therefore, this paper chooses to design a non-contact measurement system of alcohol content based on near infrared spectroscopy.

3. MATERIALS AND METHODS

3.1. Materials and equipment

Reagent: Ethanol (analytical pure, 95%): Chengdu Colon Chemical Co., LTD., the experimental water was deionized water.

Solution preparation: ethanol (analytically pure) was used as the solute, and an alcohol solution with a concentration gradient of 2% was prepared as the calibration sample, and the sample concentration range was 20%-80%.

NIRPro near infrared spectrometer: Shanghai Ruhai Optoelectronics Technology Co., LTD., detector for high sensitivity InGaAs detector, set spectrum scanning range: 950~1700 nm, integration time: 100 us, average times: 5, resolution: 8 cm-1; CVT-721 reversible quartz colorimetric dish; HL2000-P20 High power continuous Tungsten Halogen lamp: Shanghai Ruhai Optoelectronics Technology Co., LTD. QP600 multi-mode fiber; 1310 nm near-infrared laser; Special four-sided cupola support; Near infrared detector module.

3.2. Experimental Methods and Procedures

The design principle of the hardware part is: By using the characteristic absorption of near-infrared light by alcohol, a near-infrared laser of a specific wavelength is selected and the near-infrared light emitted by the laser is used to irradiate the colorimetric dish containing alcohol solution. After the near-infrared light is absorbed by the characteristic absorption of the alcohol solution in the colorimetric dish, the photodetector detects the concentration of alcohol in the solution and converts it from optical signal to current signal. The collected current signal is amplified into voltage signal by current flow voltage amplifier module. Then it is converted into digital signal by A/D converter and transmitted to the data acquisition and analysis system. Finally, the predictive regression model is calculated through PC analysis and processing, and the model is substituted into the detection system to realize and display the concentration value of the measured alcohol solution. The program design of the software design part adopts the modular design idea, and the function of each subroutine is relatively independent, which is easy to debug and modify.

Due to the characteristic absorption of alcohol solution in the near-infrared spectral band of 1310 nm, it can be used as the characteristic information to identify alcohol solution and measure the concentration of alcohol solution under normal temperature and pressure.

The non-contact alcohol measurement system is based on the characteristic absorption of alcohol solution to the near-infrared spectral band. First, the near-infrared spectrometer is used to collect the spectral characteristics of alcohol solution with different concentration gradients, and the characteristic absorption peak sensitive to alcohol solution is obtained according to the spectral analysis. The wavelength of the light source is determined according to the position and size of the spectral characteristic absorption peak. As a light source for non-contact measuring system of alcohol content.

The tungsten halide light source was preheated for 10 min, and then the empty background of the cuvets was collected by NIR spectrometer. Then the prepared alcohol samples were successively poured into the cuvets, and the spectrum of the samples was collected by transmission scanning. The spectrum scanning range was 950~1700 nm. The optical path of the quartz comparator is 10 mm, and the spectrum of the samples is collected at normal temperature, each sample is collected three times, and the computer is used as the output end of the spectrum signal acquisition software Uspectral-PLUS 6.7.0 waveform. The NIR spectra obtained by scanning the sample solution in the range of 950~1700 nm are shown in Figure 2-1:

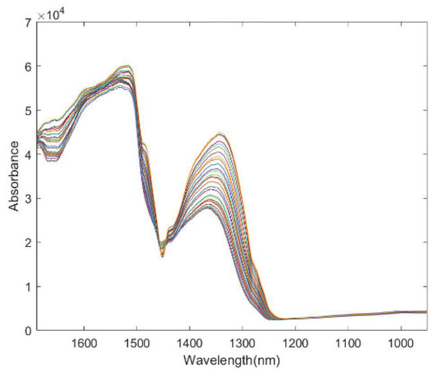

Figure 2-1 Spectra of alcohol solutions with different concentration gradients

By analyzing the spectrogram, it can be found that the NIR spectral characteristic absorption peak of the alcohol solution is mainly concentrated at the wavelength of 1350 nm. With the increase of the concentration of the alcohol solution, the absorption intensity near the wavelength of 1350 nm increases significantly compared with other wavelength positions, so it can be judged that the NIR characteristics of the alcohol solution are more obvious at this band. Based on this, a near-infrared laser with a wavelength of 1310 nm is selected as the light source, as shown in Figure 2-2:

Figure 2-2 Near infrared laser

Table 2-1 lists the main parameters of the laser.

Table 2-1 Laser configuration table

Name	Argument
Wave length	1310 nm
Output power	<5 mw
Operating voltage	2.8-3.5 V
Working current	<100 mA
Operating temperature	-20℃-+50℃
Spot size	50 MM<3 mm
Angle of divergence	<0.7 mard

The laser is a near-infrared laser with a wavelength of 1310 nm, which is convenient for the selection of other optical components. The laser has strong stability, good monochromaticity, temperature drift ±1nm, and is suitable for long-term measurement of the system. The spot diameter is 0.3mm ±0.05, the divergence Angle is < 0.7mard, and the spot diameter and divergence Angle are small, which meets the requirements of the laser spot incident on the part to be measured. Based on the above analysis, the laser is suitable for the measurement light source of this system.

4. RESULTS AND DISCUSSION

4.1. Model of The Relationship between Alcohol Solution Concentration and Voltage

Because the light intensity will be affected by the fluctuation of the light source and the influence of the external environment, the voltage ratio algorithm is used to eliminate the influence of the light intensity factor.

The relationship model between detector and alcohol solution concentration was established, the relationship between input and output model was fitted, and the fitting parameters were obtained. The prepared alcohol aqueous solution with a concentration gradient of 2% was used as the sample solution, and the sample concentration range was 20%-80%. According to the liquid sample concentration ratio, the corresponding detector measurement voltage is obtained. Some data are shown in Table 3-1:

Table 3-1 Table of alcohol solution concentration and voltmeter

Alcohol solution concentration /%vol	Voltage value
20	1.0250
30	1.0245
40	1.0230
50	1.0212
60	1.0200
70	1.0180
80	1.0175

The exponential function was used to fit the relationship between the concentration of alcohol solution and the voltage change of the photodetector, and the model of the relationship between the concentration of alcohol solution and the voltage was obtained, as shown in Figure 3-1:

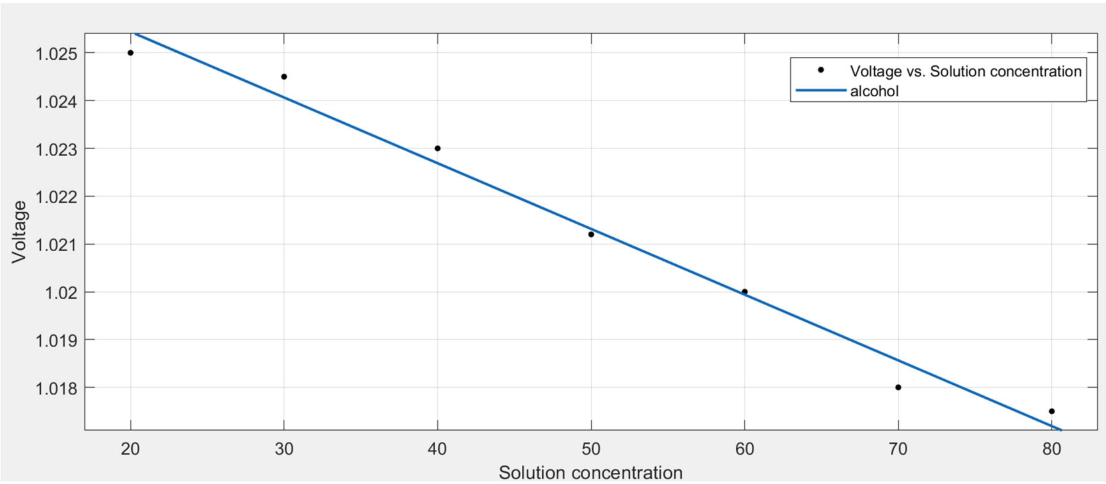

Figure 3-1 Alcohol solution concentration and voltage relationship model

As can be seen from Figure 3-1, as the concentration of alcohol liquid increases, the output of the detector becomes weaker, showing an exponential relationship, indicating that the spectral absorption of alcohol liquid follows Lamberbier's law under a stable laboratory environment. The expression of the exponential function obtained through fitting is as follows:

$$y = 1.028 \cdot e^{-6.672\times10^{-5}x} + 1.375\times10^{-9} \cdot e^{-0.05665x} \tag{2}$$

Where: y represents the voltage output of the detector after amplification and analog-to-digital conversion; x is the concentration of liquid that passes through.

The evaluation parameters of the fitted exponential function model are shown in Table 3-2:

Table 3-2 Table of model evaluation parameter

Evaluation parameter	Standard deviation	R2	Adjusted R2	Root mean square error
Numerical value	9.111×10–7	0.9831	0.9797	0.0004269

4.2. Model Revision and Evaluation

The BP neural network model is established in the MATLAB simulation program. The BP neural network model trains the model parameters by calculating the minimum root-mean-square error. The number of training steps increases while the root-mean-square error decreases continuously until the error reaches the allowable error range or exceeds the number of training steps. The learning rate of this model is 0.3, the hidden layer has 6 neurons, and the number of training steps is 64. The variation of model error with training is shown in Figure 3-2:

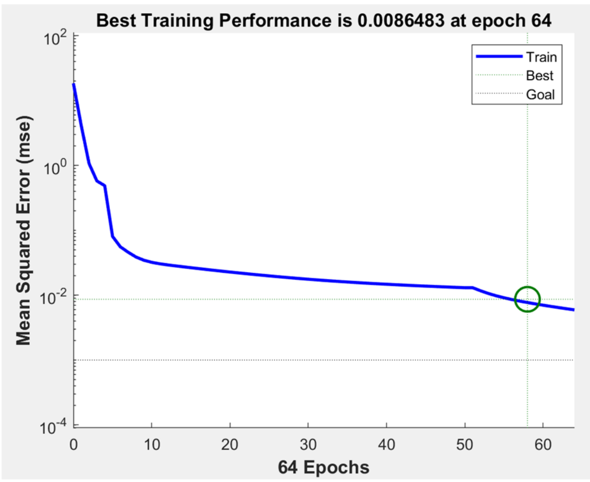

Figure 3-2 Error variation with the number of training

By analyzing the data in Table 3-3, it can be seen that the alcohol concentration predicted by the BP neural network temperature correction method is closer to the true value than that predicted by the index fitting method, and the standard deviation of the overall sample error is also smaller. The above data verify that the BP neural network temperature correction method has a better effect on the alcohol concentration prediction.

Table 3-3 Table of partial prediction error

Concentration	Exponential fitting method is used to predict concentration	BP neural network predicts concentration	Prediction error of exponential fitting method	Prediction error of BP neural network
30	21.7	26.1	8.266669052	3.920268702
30	35.4	21.6	–5.438678342	8.427306293
30	24.1	21.7	5.886509571	8.315740568
50	47.8	51.8	2.234567379	–1.766418361
50	51.0	44.4	–1.035570639	5.626445231
50	44.6	49.1	5.42093496	0.946998419
70	72.8	74.5	–2.838812408	–4.466340008
70	69.7	66.5	0.310392552	3.51272509
70	63.0	70.4	6.963089498	–0.421282919

5. CONCLUSION

In this study, two methods based on exponential function fitting model algorithm and BP neural network temperature correction algorithm are analyzed and compared in practical experiments, and the BP neural network temperature correction algorithm obtained by calculation and analysis is relatively better. By comparing the difference of the two groups of error standards, the stability and accuracy of alcohol liquid concentration prediction were improved by adding BP neural network correction algorithm, which made the non-contact measurement method based on near infrared spectrum suitable for online alcohol detection.

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