Multichannel Multicomponent Solution Concentration Detection Method based on Dual Wavelength Spectrophotometry

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Abstract: The traditional method based on stoichiometric spectrophotometry for the detection of the concentration of dye solution components cannot accurately detect the components with similar spectrum or low concentration at the same time, resulting in a low concentration range for accurate detection. In order to solve the above problems, a multichannel multicomponent solution concentration detection method based on dual wavelength spectrophotometry was studied. A spectrum detection device composed of optical fiber probe and CCD array detector is arranged and optical path calibration is carried out on the device. After processing the spectral data, the multi-channel detection of multi-component concentration was realized by using support vector machine. Compared with the two traditional methods, the experimental results show that the detection method based on dual-wavelength spectrophotometry can effectively remove interference, improve the detection range of concentration, and the detection error is within 0.3%.

Keywords: Dual wavelength spectrophotometry; Multi-component dye solution; Concentration detection; Support vector machine

1. Introduction

In the process of dyeing, the concentration of dye is the key factor that affects the color of textile. In the process of dyeing, most of the dyes used are mixed dyes. In order to determine the dyeing of a single dye in the mixed dyes, the concentration of the dye in the mixed solution or the amount of dye on the dye must be measured. There are many methods for the detection of dye concentration, including electrochemical method and optical analysis [1]. The electrochemical method is tedious in steps and takes a long time to operate, which is not conducive to the online measurement of dye concentration.

When the traditional stoichiometric method based spectrophotometry is used for the determination of dyes with similar colors, the measurement error is large when the absorption spectra of similar color components overlap seriously, the dye components are relatively large or the concentration of one dye is small compared with other components [2]. At the same time, the detection method of dye component concentration will be affected by dye properties, dyeing temperature and salt and other factors, resulting in detection errors. Based on the above analysis, a multichannel multicomponent dye concentration detection method based on dual wavelength spectrophotometry is studied in this paper.

2. Multichannel Multicomponent Solution Concentration Detection Method based on Dual Wavelength Spectrophotometry

2.1. Arrangement testing device

Dual wavelength spectrophotometry is based on Lambert-Beer law, which describes the linear relationship between the mass concentration of the dye solution and the absorption of the dye solution under certain conditions. The two wavelengths were sequentially passed through the tested dye solution containing various components. It was assumed that the tested components of the dye solution met the Lambert-Beer law at the two wavelengths, and the following equation existed [3].

$$\Delta A = A_1 - A_2$$
$$= \left(\varepsilon_{11} - \varepsilon_{12}\right)b \bullet c_{x1} + \cdots + \left(\varepsilon_{i1} - \varepsilon_{i2}\right)b \bullet c_{xi} \quad (1)$$

In formula (1), ε_{i1} and ε_{i2} respectively represent the light absorption coefficients of the measured component x_i under detection wave λ_1 and λ_2, b represents the light diameter length of the measured dye solution. c_{xi} represents the mass concentration of component x_i of the dye tested. According to the above principle, the optical fiber spectrometer composed of the optical fiber probe and CCD array detector was selected to detect the concentration of the components of the dye solution. The following figure is a schematic diagram of the arrange-

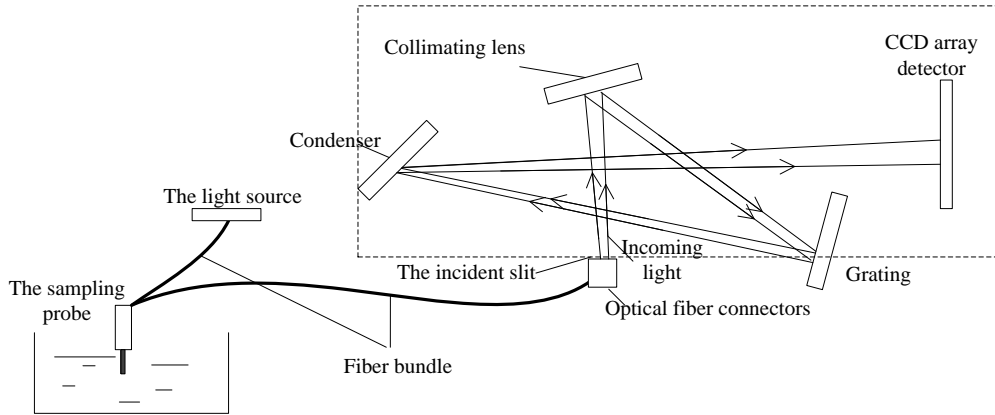ment of optical fiber spectrometer using optical fiber probe and array detector.

Figure 1. Schematic diagram of arrangement of detection device

It is necessary to calibrate and adjust the light path of the spectrometer after arranging the dye component detection device. After calibration and adjustment, the spectrum spectrometer will send the obtained dye solution spectrogram of each component to the upper computer, and conduct data analysis in the upper computer to determine the concentration of each component.

2.2. Optical path calibration of detection device

In order to obtain a certain monochromatic light, the grating must be rotated at a certain Angle. The diagram below shows the optical structure of chernitna system [4].
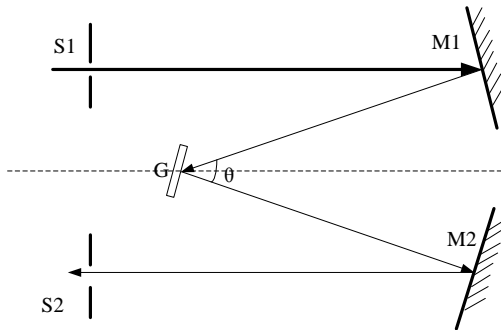

Figure 2. Schematic diagram of optical structure of chernitna system

Adjust the optical path of the spectrometer according to the following steps:
a. According to the optical path structure shown in figure 2, the incident slit and the exit slit, the collimating mirror and the focusing mirror as well as the grating are installed at the appropriate position of the device platform, and the center height between them is adjusted at the same height.
b. Calibration collimator M1: put a light source in the position of the incident slit, and the light will be incident from the incident slit to the collimator M1. At this time,

the position of M1 is adjusted back and forth. When the image formed by M1 is roughly the same as that of the incident slit and clear, it indicates that the incident slit S1 is on the focal plane of the collimator M1. Then adjust the pitch Angle of M1 to make the imaging height consistent with the height of the slit, rotate M1 to make the imaging above the grating, and then fix the M1 position.
c. Adjustment of grating: after the light passes through M1, the light that reaches the grating G is the parallel light to adjust the elevation Angle of the grating, so that the diffraction light is equal to the incident slit in height. Then rotate the grating G to make the light shine on the concentrator M2.
d. Adjustment of concentrator M2: rotate M2 to make the diffraction light reach the exit slit, and adjust the position of M2 before and after. When the light intensity is maximum at exit slit S2, the S2 position is fixed. After the above four steps of light road construction and adjustment has been completed. After adjusting the optical path, the wavelength of the detection light is calibrated. The known grating equation is as follows:

$$d \sin \theta_1 - d \sin \theta_2 = m\lambda \qquad (2)$$

In formula (2), d is the distance between the marks of the grating. θ_1 and θ_2 are incident and diffraction angles relative to the normal line of the grating respectively. m is the diffraction order and λ is the diffraction wavelength [5]. The above formula can be obtained by mathematical transformation of trigonometric functions:

$$\begin{cases} 2d \cos \beta \sin \alpha = m\lambda \\ \dfrac{\theta_1 + \theta_2}{2} = \beta \\ \dfrac{\theta_1 - \theta_2}{2} = \alpha \end{cases} \qquad (3)$$

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Since the incident slit and the outgoing slit have been fixed, half β of the sum of the incident Angle and the outgoing Angle is a fixed value. When the grating rotates the incident light remains unchanged, the Angle of the outgoing light is twice that of the grating, so α represents the Angle of the grating [6-7]. After adjusting and calibrating the light path of the spectrophotometer, the dye component spectrum obtained by the spectrometer was analyzed and processed in the upper computer.

2.3. Spectral data processing

Visible spectral data in visible spectral analysis are usually represented by vectors and matrices. For a sample of visible spectral data with L spectral data, the corresponding wavelength vector is $\mu_1, \mu_2, \mu_3, \ldots, \mu_l$, and the corresponding absorbance vector is $\chi_1, \chi_2, \chi_3, \ldots, \chi_l$. For n groups of visible spectrum data samples, the following absorbance matrix X_{nl} is used to represent:

$$X_{nl} = \begin{bmatrix} \chi_{11} & \chi_{12} & \cdots & \chi_{1l} \\ \chi_{21} & \chi_{22} & \cdots & \chi_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_{n1} & \chi_{n2} & \cdots & \chi_{nl} \end{bmatrix} \quad (4)$$

Each sample has the visible spectrum data sample of m components, which can be represented by the following component concentration matrix Y_{nm}:

$$Y_{nm} = \begin{bmatrix} y_{11} & y_{12} & \cdots & x_{1m} \\ y_{21} & y_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{bmatrix} \quad (5)$$

The sample set can be expressed as $\{(x_i, y_i), i = 1, \cdots, n\}$, and the normalization of the sample can reduce the influence of noise and drift, and improve the accuracy and resolution of the analysis of mixed dye components [8]. In this paper, the spectral data are preprocessed by the method of data normalization expansion. The value of the normalized data is 0 ~ 1. The extension is to enlarge the spectral data, so as to facilitate the support vector machine algorithm to carry out detailed processing of the minor changes of spectral data, so as to improve the resolution and accuracy of the analysis. The normalized extension can be expressed in the following formula:

$$\begin{cases} x_i' = \dfrac{x_i}{x_a} \times K \\ x_a = \dfrac{1}{q} \sum\limits_{i=1}^{q} x_i \end{cases} \quad (6)$$

In formula (6), x_i' is the spectral data after normalization, x_i is the spectral data before normalization, x_a is the average value of mixed dye spectral data, q is the number of spectral data, and K is the amplification factor [9]. After processing the spectral data, support vector machine algorithm was used to detect the multi component concentration of dye solution simultaneously.

2.4. Multi - channel detection concentration is realized by SVM technique

Support vector machines can maximize the complexity of SVM classifier by maximizing the classification interval, so as to achieve good generalization ability. For the linear inseparability problem, SVM adopts the method of mapping the original space of data to the feature space of high dimension, and minimizes the structural risk by finding the optimal hyper plane in the feature space of high dimension. At the same time, the kernel function is used to transform the nonlinear operation of the original space into the inner product operation of the high-dimensional feature space. The classification decision function is as follows:

$$f(x) = \text{sgn}\left\{ \sum_{i=1}^{n} X_i^* \times y_i(x) + \delta^* \right\} \quad (7)$$

In formula (7), X_i^* is the classification sample data, $y_i(x)$ is the spectral data of the dye components to be detected, and δ^* is the classification threshold of support vector machine. The threshold value is determined according to the training results [10]. Support vector machines are trained with component concentration samples. The dye spectrum data with known component concentration was selected as the training sample, and the support vector machine was trained according to the following process.
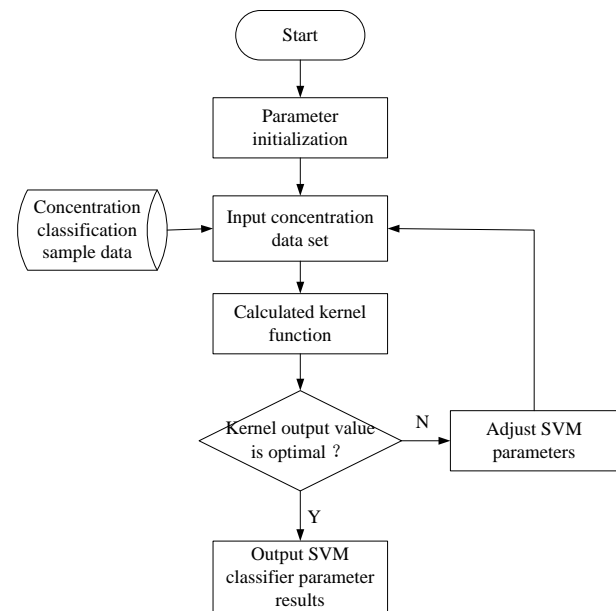

Figure 3. Training flow chart of support vector machine

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When the SVM classifier meets the optimal classification decision function, the detection of component concentration is completed and the corresponding detection results are output. The above research has been done on the multi-channel multi-component dye concentration detection method based on dual-wavelength spectrophotometry.

3. Experiment

In this paper, a multi-channel multi-component dye concentration detection method based on dual-wavelength spectrophotometry is studied. In order to verify the feasibility and effectiveness of the method and test the performance of the detection method in the detection of concentration, this section will design relevant verification experiments, through the analysis of experimental data, to complete the preset verification objectives.

3.1. Experiment content

This experiment as the contrast experiment, experiment contrast group 1 is the concentration of dyeing liquid detection method based on the absorption spectrum area, control group 2 based on partial least squares method of

spectrophotometric dye solution concentration detection method, the experimental group for this study based on dual wavelength spectrophotometry of multi-channel multicomponent dye solution concentration detection method. The test object is the dye solution of different component concentration configured in a certain proportion. The dye solution group used in the experiment is divided into three solid reactive dyes: red, yellow and blue. The experimental comparison index is the relative error value of the detection method for the concentration of three components in the dye solution and the concentration range that can be accurately determined by the method. By comparing the above two indicators to measure the performance of the three detection methods in the comparison group and the experimental group, the feasibility of the detection method studied in this paper was verified.

3.2. Experiment preparation

The method of mother liquor dilution was used to reduce the weighing error. Related equipment and parameters of dye preparation are shown in the following table:

Table 1. Dye preparation related equipment and parameters

Configuration of equipment	Parameter	Quantity
Analytical balance	Model: FA2004, range: 0.1mg	2
Quartz colorimetric dish	Optical path :12.5 mm	90
Volumetric flask	25ml/50ml/100ml/250ml/500ml/1000ml	30 for each specification
Beaker	100ml/500ml	20 for each specification
Pipette	1ml/2ml/5ml/10ml	15 for each specification
Measuring cylinder	50ml/100ml	30 for each specification
Glass agitator	—	30

After the experimental solution was configured, the composition concentration of the experimental solution was determined by using three methods: the contrast group and the experimental group. The test will be experimental data input MATLAB. Analyze and process the experimental data, compare the experimental indexes of the three methods, and draw the experimental conclusion.

3.3. Experimental results

The test results of the dye concentration of the experimental solution by three methods in the comparison group and the experimental group are shown in the following table. Analyze the data in the table and draw corresponding conclusions.

Table 2. Test results of group method 1

Solid with concentration (10-3g/L)			Concentration ratio	Detection of concentration (10-3g/L)			Relative error /%		
Red	Yellow	Blue		Red	Yellow	Blue		Red	Yellow
50	1.25	1.25	40:1:1	52.221	1.424	1.078	-2.221	-0.174	0.172
50	50	1	50:50:1	47.691	50.312	1.177	2.309	-0.312	-0.177
0.556	50	0.556	1:90:1	0.456	51.247	0.697	0.1	-1.247	-0.141
2.5	50	50	1:20:20	2.28	47.023	53.47	0.22	2.977	-3.47
0.625	0.625	50	1:1:80	0.534	0.793	54.934	0.091	-0.168	-4.934
50	0.714	50	70:1:70	53.297	0.579	48.067	-3.297	0.135	1.933

Table 3. Test results of group method 2

Solid with concentration (10-3g/L)			Concentration ratio	Detection of concentration (10-3g/L)			Relative error /%		
Red	Yellow	Blue		Red	Yellow	Blue		Red	Yellow
50	1.25	1.25	40:1:1	48.191	1.392	1.424	1.809	-0.142	-0.174
50	50	1	50:50:1	48.364	50.009	1.01	1.636	-0.009	-0.01
0.556	50	0.556	1:90:1	0.423	46.398	0.531	0.133	3.602	0.025
2.5	50	50	1:20:20	2.34	47.361	52.314	0.16	2.639	-2.314

| 0.625 | 0.625 | 50 | 1:1:80 | 0.593 | 0.573 | 46.746 | 0.032 | 0.052 | 3.254 |
| 50 | 0.714 | 50 | 70:1:70 | 55.931 | 0.899 | 54.631 | -5.931 | -0.185 | -4.631 |

Table 4. Test results of the experimental group

Solid with concentration (10-3g/L)			Concentration ratio	Detection of concentration (10-3g/L)			Relative error /%		
Red	Yellow	Blue		Red	Yellow	Blue	Red	Yellow	Blue
50	1.25	1.25	40:1:1	49.991	1.249	1.251	0.009	0.001	-0.001
50	50	1	50:50:1	50.102	50.009	1.010	-0.102	-0.009	-0.01
0.556	50	0.556	1:90:1	0.54	49.973	0.546	0.016	0.027	0.01
2.5	50	50	1:20:20	2.37	50.241	50.148	0.13	-0.241	-0.148
0.625	0.625	50	1:1:80	0.631	0.620	50.247	-0.006	0.005	-0.247
50	0.714	50	70:1:70	49.768	0.702	49.837	0.232	0.012	0.163

The analysis of the above 3 Tables shows that the detection of high concentration of one component and low concentration of the other two groups of dye solution: the error of detection of high concentration of the two groups was greater than that of the experimental group. For the detection of two low-concentration components, the two methods in the comparison group had the largest error in the detection of high-concentration components, followed by the comparison group method 1. For high concentration of two components and low concentration of the other group, the detection error of method 2 in the comparison group was less than that in the comparison group and greater than that in the experimental group. The detection error of the comparison group was greater than that of the experimental group. The relative error of the experimental group was within ±0.3%. The above data indicate that the experimental group method can more accurately detect the components with similar concentrations.

The range of dye concentration accurately detected by the three methods is shown in the following figure.
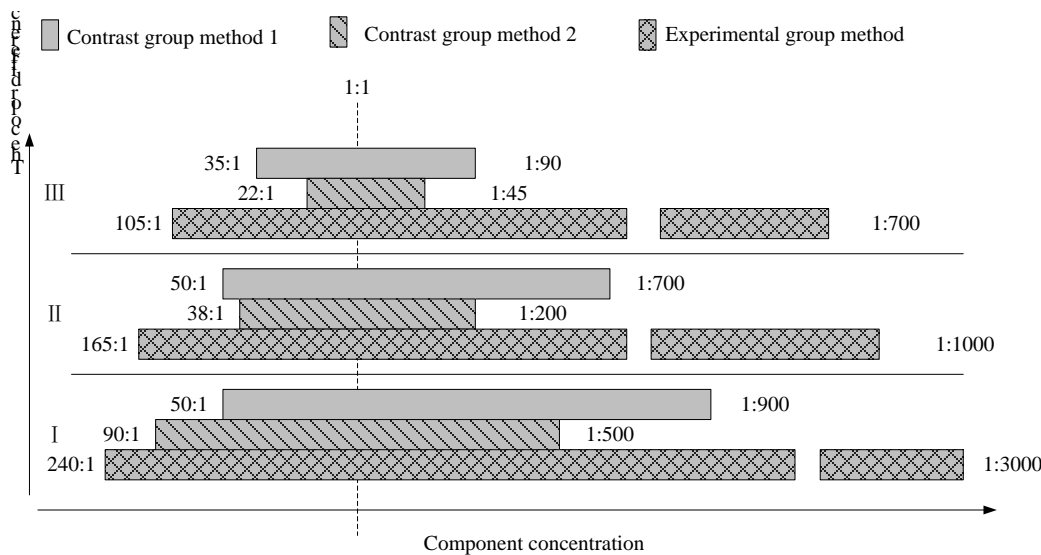

Figure 4. Accurate detection ranges of the three methods

It can be seen from the above figure that with the increase of color difference level, the accurate detection range of the two methods in the comparison group for multiple components of the dye solution was gradually reduced, while that of the experimental group was less. To sum up, the multi-channel multi-component solution concentration detection method based on dual-wavelength spectrophotometry studied in this paper can detect the multi-component solution more accurately, and the accurate detection range is larger.

The traditional spectrophotometry can only detect the fuel concentration with a large color difference. In order to accurately detect the concentration of the fuel with a similar color, a multi-channel multi-component dye concentration detection method based on dual-wavelength spectrophotometry was studied in this paper. By comparing with two kinds of concentration detection methods, it is proved that the detection method can effectively improve the detection accuracy of the concentration of dye solution and has practical application value.

4. Conclusion

5. Acknowledgments

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