

Based on multi-characteristic spectral non-contact quantitative detection system for sugar content

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To achieve non-contact quantitative testing of various sugar-like concentrations in sugar-sweetened beverages, we built an infrared spectroscopy testing system for sugar-sweetened beverages, and proposed a multi-characteristic spectral weighting algorithm. The system uses the infrared laser to irradiate sugar-sweetened beverages and analyzes their absorption characteristics in the reflected spectrum. We selected multi-characteristic wavelengths for combined analysis based on the characteristic wavelength distribution of the sugar. In the calibration experiment, it obtained the near-infrared characteristic spectrum distributions of glucose, sucrose, and fructose. During the process of changing sugar concentration from 1.0% to 5.0%, the absorbance increased from 0.045 to 0.215. The linearity of its growth rate is 0.997. The test results for comparing algorithms show that in condition 1, the SCW method's test mean is very different from the real value. It cannot tell the difference between different types of sugar concentrations in mixed sugar solutions. The test mean of the DWD method and this algorithm are 19.1% and 6.3%, respectively. In condition 2, the test mean values of SCW method, DWD method, and this algorithm are 15.0%, 7.6%, and 4.2%, respectively. It verifies that this algorithm has better accuracy in sugar concentration inversion.

Keywords: sugar concentration, multi-characteristic spectrum, weighted algorithm, non-contact detection.

1. Introduction

Sugar-sweetened beverages play an important role in helping athletes quickly replenish energy [1]. When the sugar content is too low, it is difficult to achieve the effect of supplementing energy. When the sugar content is too high, it can cause significant fluctuations in blood sugar, leading to fatigue and affecting exercise performance. Blood sugar has a certain impact on heart rate changes and exercise status [2,3]. Therefore, it is of great significance to quantitatively detect the sugar types and contents of sugar-sweetened beverages.

The traditional chemical testing method requires contact with the sample, and the quantitative detection steps are complex and time-consuming. On the other hand, using a certain wavelength of infrared laser to shine on the sample and figure out the pro-

portion of characteristic spectrum can keep the drink from getting contaminated again. And the use of multi-characteristic spectral inversion algorithm can achieve rapid quantitative identification of various sugars. LI *et al.* [4] used near-infrared spectroscopy to test the content of sugar and glutinous rice flour in green tea and used an iterative algorithm to build a support vector machine model. The recognition rate was better than 97%, and the prediction correlation coefficient was 0.94. XIAO *et al.* [5] used THz spectroscopy to determine the content of sugar and potassium sorbate in milk powder. The target recognition rate for powdered samples was 90%, but the quantitative accuracy was not high. WANG *et al.* [6] used time-domain THz scanning technology to test anhydrous glucose. Although THz spectroscopy technology has the advantages of high accuracy and fast speed, it is not suitable for detecting sugar content in sugary drinks because water can strongly absorb THz light. NING [7] used infrared characteristic spectroscopy to test the sucrose content in sucrose juice, with an accuracy of better than 1.2%, but could only identify a single type of sugar. LIEBMANN *et al.* [8] used the infrared transmission method to invert the concentrations of glucose and alcohol and the accuracy of glucose concentration detection is about 4.5%. ZHAO *et al.* [9] used spectral analysis of diffuse reflectance light from fruits to achieve non-destructive detection of fruit sugar content and its detection accuracy is about 3.7%. LÜ *et al.* [10] studied the inversion results of sucrose transmission spectra at three different testing angles, and found that the sucrose content prediction model had the best performance under 120° conditions, verifying the role of spectral modulation in sugar inversion. TANG *et al.* [11] used a wide spectrum of 350–1075 nm to test sucrose content, and their segmented PLS model for sugar inversion showed greater stability. PHUPHAPHUD *et al.* [12] designed a portable visible short infrared combined spectral detection system, which showed the best suppression effect on external skin interference. CHEN *et al.* [13] used diffuse reflectance spectroscopy to predict the sugar content of cherries, and the correlation coefficient of the test set reached 0.83. CHEN *et al.* [14] constructed a PLS model using Fourier transform near-infrared spectroscopy for sugar content testing of kiwi-fruit. In addition, some studies have used various types of lasers [15–17] as light sources for testing. In the testing process, lasers are not used for different characteristic wavelengths.

Previous papers studies have mainly focused on the quantitative identification of single sugar types. There are few reports on the quantitative detection of sugars in sugar-sweetened beverages. The mixed spectrum recognition method of visible light and infrared light can demonstrate that the inversion of multiple characteristic spectra is useful for multi-component recognition and improving the accuracy of sugar content detection. Therefore, this article proposes a sugar concentration inversion algorithm for non-contact multi-component quantitative detection of sugar-sweetened beverages.

2. System design

To get quick results and keep the sample from getting contaminated, we designed a method for inverting the sugar concentration of sugar-sweetened beverages by combining

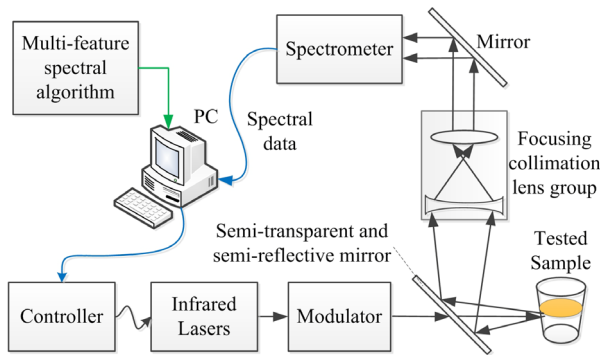


Fig. 1. Sugar concentration detection system based on multi-characteristic spectrum algorithm.

multi-infrared characteristic absorption peaks. By changing the infrared laser's energy output [13, 14], the system scans separately for the characteristic peaks of different sugars. It then uses a spectrometer to extract multi-characteristic spectrum, which lets it measure the amounts of multiple sugars and figure out what they are. Figure 1 illustrates the non-contact sugar concentration detection system for sugar-sweetened beverages.

The computer controls the module to emit infrared laser signals. When the module is modulated, an infrared laser light source [15] is given carrier signals at several characteristic wavelength positions. This makes it easier to pick up these signals during the demodulation process. The testing distance is set between 10 and 15 cm. The distance between the incident mirror and the surface of the sugar water is within this range. The incident light is directed onto the test sample through a semi-transparent and semi-reflective mirror. The test sample's light is reflected by a half mirror and sent to a group of convergent collimating lenses. These lenses shape the beam into parallel light. The shaped beam is collected and analyzed by a spectrometer, and the obtained spectral data is imported into a computer. We determine the types and concentrations of sugars in the test sample using a multi-characteristic spectral algorithm. Then we compare the inverted data with common carbohydrate enzyme coupling methods to verify the feasibility and accuracy of the system.

3. Model construction and algorithm design

3.1. Sugar concentration inversion model

Due to the different molecular structures of different types of sugars, their ability to absorb light of different wavelengths varies greatly. In this system, the analysis mainly focuses on glucose, sucrose, and fructose. Laser modulation can still be used to test a part for multi-feature spectral inversion models as long as it has clear spectral characteristics, even if some of its characteristic wavelengths overlap. If sugars A, B, and C will be tested, each type can be classified into three levels (1, 2, and 3) based on the absorption intensity of their spectral absorption peaks. This results in three groups of

characteristic spectral data: A (A1, A2, A3), B (B1, B2, B3), and C (C1, C2, C3). If there are more types of sugars, corresponding letters can be set according to the actual types of sugars to represent the corresponding types of sugars, such as D, E, and so on. After that, inversion is used to fully identify and quantify the different types of sugars in sugary drinks based on the different contributions of characteristic wavelengths to the absorption degree of different sugars.

The absorption intensity and concentration satisfy Lambert Beer's law. For the first type of A-class sugar, the changes in light intensity at the three characteristic wavelength positions can be expressed as

$$\begin{cases} I(\lambda_{A1}) = I_0(\lambda_{A1}) \exp[-\alpha(\lambda_{A1})C_A h + \beta] \\ I(\lambda_{A2}) = I_0(\lambda_{A2}) \exp[-\alpha(\lambda_{A2})C_A h + \beta] \\ I(\lambda_{A3}) = I_0(\lambda_{A3}) \exp[-\alpha(\lambda_{A3})C_A h + \beta] \end{cases} \quad (1)$$

Among them, $I(\lambda_{A1})$ represents the reflected light intensity at the wavelength λ_{A1} ; $I_0(\lambda_{A1})$ represents the initial light intensity at the position of wavelength λ_{A1} ; λ_{A1} , λ_{A2} , and λ_{A3} represent the three characteristic wavelength values with the highest absorbance of A-class sugars; $\alpha(\lambda)$ represents the absorption coefficient at the corresponding wavelength. These coefficients are different for the different characteristic wavelengths; C_A represents the concentration of A-class sugars; h represents the depth of illumination; and β is the interference coefficient of the optical system. The deformation of formula (1) includes

$$C_A = \frac{1}{\alpha(\lambda_{Ai})h} \left[\ln |I(\lambda_{Ai}) - I_0(\lambda_{Ai})| - \beta \right] \quad (2)$$

Among them, $i = 1, 2, 3$. In theory, the C_A inverted at any feature position is the same, but in reality, due to the different absorption levels at the feature wavelength position, the absorption levels of other solutes in the same solution at that wavelength position are also different. Therefore, the C_A calculated by λ_{A1} , λ_{A2} , and λ_{A3} will also differ. Therefore, weighted averaging of test results for multi-characteristic peaks can improve the accuracy of concentration calculation.

For class B and C sugars, formula (1) also applies. These parameters based on characteristic spectral absorption form the inversion dataset, and their relationship with the concentrations of the three sugars is as follows:

$$\begin{bmatrix} C_A \\ C_B \\ C_C \end{bmatrix} = \begin{bmatrix} I(\lambda_{A1}) & I(\lambda_{A2}) & I(\lambda_{A3}) \\ I(\lambda_{B1}) & I(\lambda_{B2}) & I(\lambda_{B3}) \\ I(\lambda_{C1}) & I(\lambda_{C2}) & I(\lambda_{C3}) \end{bmatrix} \begin{bmatrix} k_1 \\ k_2 \\ k_3 \end{bmatrix} \quad (3)$$

Among them, C_A , C_B , and C_C represent the concentrations of A-class, B-class, and C-class sugars, respectively; k_1 , k_2 , and k_3 represent compensation coefficients, respectively. The compensation coefficient significantly contributes to the accuracy of calculating the sugar concentration of each component.

The sugar-sweetened beverages were tested to contain several types of sugar. When Eq. (3) is calculated, the concentration inversion of different types of sugar is affected by their unique characteristic wavelengths. Therefore, it is necessary to set different weights based on the position of different characteristic wavelengths. The weight parameters are set according to different types of sugars, including

$$\begin{cases} a_1 + a_2 + \dots + a_i = 1 \\ b_1 + b_2 + \dots + b_i = 1 \\ c_1 + c_2 + \dots + c_i = 1 \end{cases} \quad (4)$$

Then Eq. (3) is transformed into

$$\begin{bmatrix} C_A \\ C_B \\ C_C \end{bmatrix} = \begin{bmatrix} a_1 I(\lambda_{A1}) & a_2 I(\lambda_{A2}) & a_3 I(\lambda_{A3}) \\ b_1 I(\lambda_{B1}) & b_2 I(\lambda_{B2}) & b_3 I(\lambda_{B3}) \\ c_1 I(\lambda_{C1}) & c_3 I(\lambda_{C2}) & c_3 I(\lambda_{C3}) \end{bmatrix} \begin{bmatrix} k_1 \\ k_2 \\ k_3 \end{bmatrix} \quad (5)$$

3.2. Multi-characteristic spectrum weighting algorithm design

Both glucose and sucrose exhibit absorption peaks in the near-infrared range of 600–1600 nm. These absorption peaks cannot uniquely calculate the concentration of a particular sugar, as they overlap with each other. Additionally, the solution is water, which has a strong absorption capacity in this wavelength range. So the error in calculating solely based on the absorption of light intensity at a certain characteristic wavelength is relatively large. We have designed an inversion algorithm based on multi-characteristic spectrum weighting. The main idea of the algorithm is to utilize the different absorption degrees of different sugars at different feature wavelength positions so as to assign different weights to different characteristic wavelength positions when inverting a certain sugar concentration. The basis for assigning weights is that different sugars have different absorption abilities for different wavelengths. Therefore, for different characteristic wavelengths, the specific gravity of a certain sugar component is different. The algorithm can achieve the inversion of sugar concentration by assigning a combination of weights. In this way, other sugars and water won't get in the way of the concentration inversion as much.

Implementation steps of multi-characteristic spectrum weighting algorithm:

(a) Select appropriate characteristic wavelength values based on the type of sugar being measured. When the number of mixed sugar types is less than or equal to 3, it is

usually possible to set 3 characteristic wavelengths for each type of sugar, which are the spectral data sets: A (A_1, A_2, A_3), B (B_1, B_2, B_3), and C (C_1, C_2, C_3).

(b) Perform sugar concentration calibration experiments based on the selected characteristic wavelengths, with a minimum detection accuracy of 1.0% for concentration. To use formula (1) to flip the concentration values of the three wavelengths (λ_A, λ_B , and λ_C), and the light intensity absorption values are inverted to obtain the sugar concentration values: C_A, C_B , and C_C .

(c) The sugar enzyme coupling method was employed to measure the sugar concentration in the same monomer sugar solution, and the test data were C_{A0}, C_{B0} , and C_{C0} . Subtract the test concentration from step (b) to obtain the compensation coefficient k_1, k_2 , and k_3 .

(d) Spectral sampling of sugar-sweetened beverages mixed with multiple sugars to obtain their near-infrared spectral data. It is possible to get two sets of light absorptivity at the characteristic peak position and the wavelength positions next to it with a small interval by using a modulation module to sweep the frequency at the characteristic wavelength position. The light absorption test results for type A sugar are used to get the weighted values of the absorption intensity set [$I(\lambda_{A1}), I(\lambda_{A2}), I(\lambda_{A3})$]. These are $[a_1 I(\lambda_{A1}), a_2 I(\lambda_{A2}), a_3 I(\lambda_{A3})]$, where $a_1 + a_2 + a_3 = 1$.

(e) Apply step (d) to species B and C to complete the acquisition of ownership values for the three types of sugars.

(f) Substitute the weight data and compensation absorption into Eq. (5) to obtain C_A, C_B , and C_C . The program flow is shown in Fig. 2.

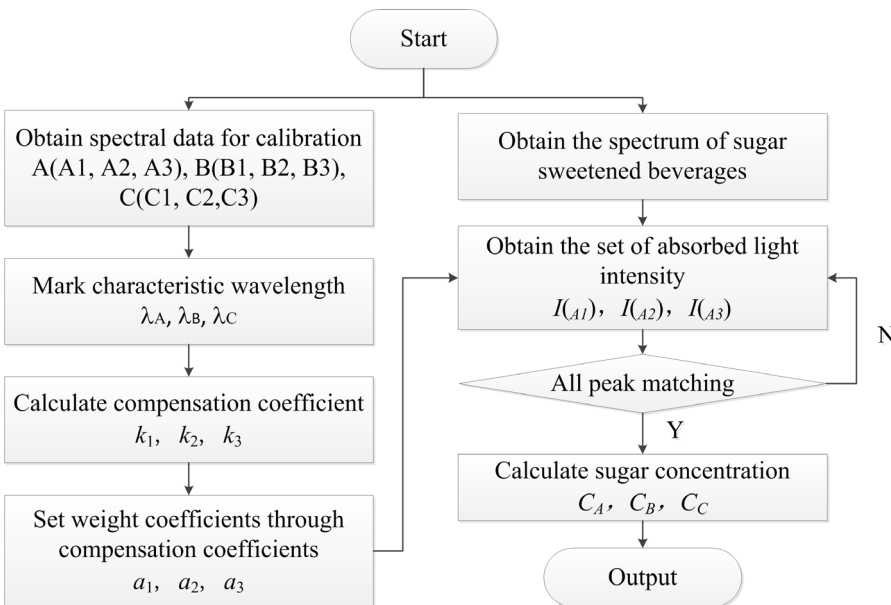


Fig. 2. Program flowchart of multi-characteristic spectral weighting algorithm.

4. Experiments

4.1. Calibration experiment

To quantitatively calculate the concentration of various types of sugars in sugar-sweetened beverages, it is first necessary to obtain the absorbance of a single sugar at several characteristic wavelengths. The calibration experiment uses glucose as a test example. The test concentrations were 0%, 1.0%, 2.0%, 3.0%, 4.0%, and 5.0%, respectively. The results of the light absorption test are shown in Fig. 3.

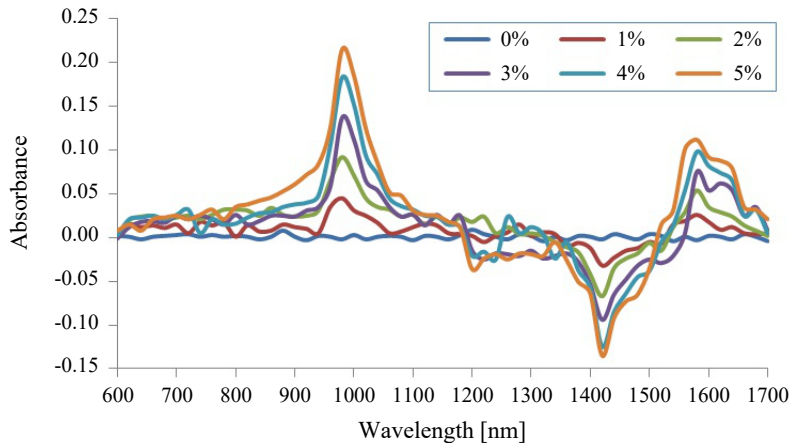


Fig. 3. Absorption spectra of glucose solutions with different concentrations in the near-infrared band.

Firstly, in order to reduce the spectral interference of solution water on solute sugars, pure water solution was used as the background spectrum for differential calculation. Pure water was used as the solution during the testing process. Test the absorption spectrum of water at the characteristic wavelength position corresponding to the sugar to be tested. Then, use the spectrum of mixed solutions with different sugar concentrations as the test spectrum. Calculate the difference between the absorbance of the test spectrum and the absorbance of the background spectrum to obtain the absorption spectrum curve of the sugar, as shown in Fig. 3. Within the near-infrared wavelength range of 600–1700 nm, glucose exhibits three distinct absorption peaks. Two positive absorption peaks are at 995 and 1560 nm, and one negative absorption peak is at 1430 nm. Among them, the absorption effect is strongest at the 995 nm position, and the absorbance increases from 0.045 to 0.215 during the change of sugar concentration from 1.0% to 5.0%. The linearity of its growth rate is 0.997, which can well reflect the degree of sugar content change within the testing interval. As the absorbance increases, the entire spectrum increases almost proportionally, so the weights do not need to be assigned to each test spectrum, but rather to the calibrated test spectrum. For sucrose and fructose, the same spectral testing calibration can obtain their corresponding char-

acteristic absorption peaks. The characteristic absorption peak of sucrose is near 220 nm. There are also small absorption peaks in the visible region, such as 684 and 758 nm. In the process of sugar concentration changing from 1.0% to 5.0%, the absorbance increased from 0.015 to 0.027. For fructose, its strongest characteristic absorption peak is around 480 nm. In the process of sugar concentration changing from 1.0% to 5.0%, the absorbance increased from 0.011 to 0.019.

4.2. Spectral acquisition experiment with different concentration ratios

To achieve quantitative detection of different types of sugar mixture solutions, it is necessary to calibrate the test values of several typical sugar mixture ratios, and then analyze the validation set through their data distribution characteristics. In the experiment, a 100 W high-power PG64623 broadband light source was used as the infrared light source. The detector adopts the 6362D spectrometer from Microphtons Technology, with a spectral scanning range of 600–1700 nm and a spectral resolution of ± 0.1 nm.

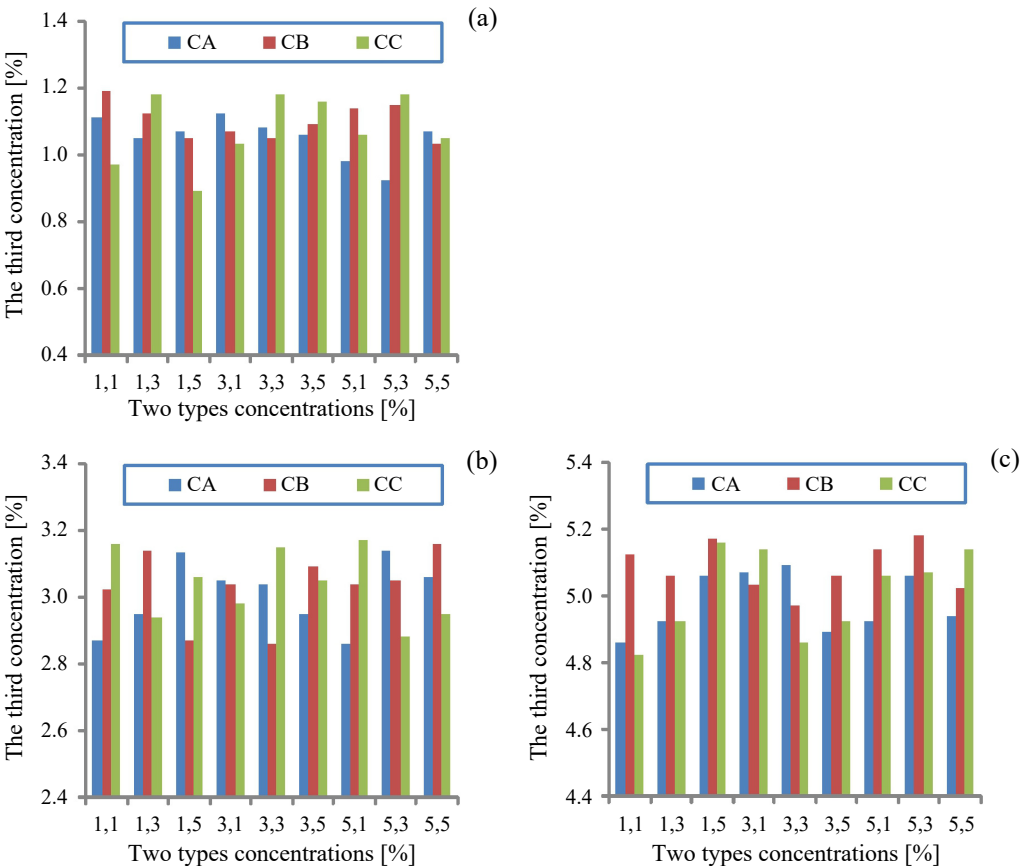


Fig. 4. Inversion concentrations in sugar solutions with different mixing ratios: (a) 1.0% (b) 3.0%, and (c) 5.0%.

Glucose is used as class A sugar, sucrose as class B sugar, and fructose as class C. Mixing ratios of 1.0%, 3.0%, and 5.0% were used to obtain a total of 27 mixed solutions for testing. After inverting the sugar concentration of 27 test solutions, the test results are shown in Fig. 4.

As shown in Fig. 4, when two sugars have concentrations of 1%, 3%, or 5%, they produce a total of 9 combinations. They are (1,1), (1,3), (1,5), (3,1), (3,3), (3,5), (5,1), (5,3), and (5,5), respectively. They correspond to the 9 cases of the horizontal axis in the figure. At this point, the concentration of the third type of sugar inverted by the multi-characteristic spectrum weighting algorithm is shown on the vertical axis in the graph. As shown in Fig. 4(a), when the true value of A-class sugar concentration is 1.0%, the inverted values of A-class sugar concentration under 8 test conditions are represented by blue bars. The maximum error is 0.12%, and the average error is 0.051%. Similarly, the maximum error of the inversion value of B-class sugar concentration is 0.19%, and the average error is 0.098%. The maximum error of the inversion value of C-class sugar concentration is 0.18%, and the average error of the true value is 0.078%. Figures 4(b) and (c) show the test results of the third sugar at concentrations of 3.0% and 5.0% for the first two sugars, respectively. When the true values of A-class sugar concentration are 3.0% and 5.0%, their test mean values are 3.05% and 4.96%. When the true values of B-class sugar concentration are 3.0% and 5%, their test mean values are 3.09% and 5.08%. When the true values of C-class sugar concentration are 3.0% and 5.0%, their test mean values are 3.04% and 5.02%. It shows that using a multi-characteristic spectrum weighting algorithm, each sugar concentration can be turned around in different combinations of different sugar concentrations.

4.3. Comparative analysis of test data

Comparative tests were done using the single characteristic wavelength (SCW) method, the dual wavelength difference (DWD) method, and the multi-characteristic wavelength weighted (MCWW) method to make sure that this algorithm worked well for solving different kinds of sugar concentrations. Each test ensures sufficient spectral stability, reducing the error caused by instantaneous detection during testing. The concentration ratios of glucose, sucrose, and fructose in the mixed sugar solution were tested for case 1 (1.0%, 1.0%, 1.0%) and case 2 (1.0%, 3.0%, 5.0%), respectively. The test results are shown in Table 1.

As shown in Table 1, under the conditions of Scenario 1, the test mean of the SCW method deviates significantly from the actual value, making it unable to detect various types of sugar concentrations in mixed sugar solutions. Under condition 2, the testing error of the three sugar concentrations has decreased slightly, but the mean is still around 15.0%. The test mean of the DWD method can basically reflect the concentration values of various sugars, and under the condition of situation 1, the average error is 19.1%. Under condition 2, the mean error is 7.6%. The test mean of the MCWW method is closer to the true value. Under condition 1, the mean error is 6.3%. Under condition 2, the mean error is 4.2%. This shows that when the MCWW method

T a b l e 1. Test results comparison for three algorithms with different mixed concentrations.

| | | Case 1 | | | Case 2 | | |
|------|----------------|--------|-------|-------|--------|-------|-------|
| | | C_A | C_B | C_C | C_A | C_B | C_C |
| SCW | Mean value [%] | 1.52 | 1.56 | 0.54 | 0.78 | 2.67 | 4.36 |
| | Error [%] | 52.0 | 56.0 | 46.0 | −22.0 | −11.0 | −12.8 |
| DWD | Mean value [%] | 1.25 | 1.27 | 0.87 | 1.12 | 3.24 | 4.89 |
| | Error [%] | 25.0 | 27.0 | −13.0 | 12.0 | 8.0 | −2.2 |
| MCWW | Mean value [%] | 1.10 | 1.09 | 0.97 | 1.06 | 3.12 | 4.92 |
| | Error [%] | 10.0 | 9.0 | −3.0 | 6.0 | 4.0 | −1.6 |

is used, the weighting effect boosts the amplitude of some characteristic wavelengths in the absorption spectrum band. It verifies the feasibility and advantages of using this algorithm. Because the purpose of testing is to detect the nutritional components of athletes' meals, more attention is paid to the average sugar concentration in sugar calculation.

5. Conclusions

This article proposes a multi-characteristic spectrum weighting algorithm for non-contact quantitative testing of sugar types and concentrations in sugar-sweetened beverages. The near-infrared spectra of glucose, sucrose, and fructose were experimentally tested, and the corresponding characteristic wavelength positions were obtained. On the basis of comparing several common sugar concentration algorithms, it was verified that this algorithm has excellent recognition for the test results of two typical sugar concentration combinations.

The main contribution of this method is the use of non-contact methods to quantitatively identify the concentrations of various sugars in mixed sugar solutions. It can be applied to beverage testing for athletes, quantitatively analyzing which type of beverage has a better effect on timely physical fitness supplementation for athletes. The application extends to the quantitative supplementation of sugar in athletes' healthy meals, offering theoretical backing for scientific meal preparation.

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