

THE DEVELOPMENT OF PORTABLE DETECTOR FOR APPLES SOLUBLE SOLIDS CONTENT BASED ON VISIBLE AND NEAR INFRARED SPECTRUM

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基于可见光和近红外光谱的便携式苹果可溶性固形物含量检测仪的研制

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ABSTRACT

In order to detect the soluble solids content of apples quickly and accurately, a portable apple soluble solids content detector based on USB2000 + micro spectrometer was developed. The instrument can communicate with computer terminal and mobile app through network port, Bluetooth and other ways, which can realize the rapid acquisition of apple spectral information. Firstly, the visible / near-infrared spectrum data and soluble solids content information of 160 apple samples were collected; secondly, the spectral data preprocessing methods were compared, and the results showed that the prediction model of sugar content based on partial least square (PLS) method after average smoothing preprocessing was accurate. The correlation coefficient (RP) and root mean square error (RMSEP) of the prediction model were 0.902 and 0.589 ° Brix, respectively. Finally, on the basis of average smoothing preprocessing, competitive adaptive reweighted sampling (CARS) and successive projections algorithm (SPA) were used to optimize the wavelength of spectral data, and PLS model was constructed based on the selected 17 characteristic wavelengths, which can increase the accuracy of soluble solids content prediction model, increase the RP to 0.912, and reduce RMSEP to 0.511 ° Brix. The portable visible / near infrared spectrum soluble solids prediction model based on the instrument and method has high accuracy, and the detector can quickly and accurately measure the soluble solids content of apple.

摘要

为了快速、准确地测定苹果可溶性固形物含量，研制了基于 USB2000+ 微型光谱仪的便携式苹果可溶性固形物含量检测仪。该仪器可以通过网络端口、蓝牙等方式与计算机终端和移动应用程序进行通信，实现苹果光谱信息的快速采集。首先采集了 160 份苹果样品的可见光/近红外光谱数据和可溶性固形物含量信息；其次，对光谱数据预处理方法进行了比较，结果表明，经过平均平滑预处理后，基于偏最小二乘法 (PLS) 的糖含量预测模型是准确的。预测模型的相关系数 (RP) 和均方根误差 (RMSEP) 分别为 0.902 和 0.589°Brix。最后，在平均平滑预处理的基础上，采用竞争自适应重加权采样 (CARS) 和连续投影算法 (SPA) 对光谱数据的波长进行优化，并根据选取的 17 个特征波长构建了 PLS 模型，提高了可溶性固形物含量预测模型的精度，使 RP 提高到 0.912，RMSEP 降低到 0.511°Brix。基于该仪器和方法的便携式可见/近红外光谱可溶性固形物预测模型具有较高的精度，该检测仪能够快速、准确地测定苹果可溶性固形物含量。

INTRODUCTION

Apple is one of the most popular fruits (LiYan Gong et al, 2014) in China. Its internal soluble solids (BRIX) directly affect consumers' willingness to buy (Fernando Mendoza et al, 2011; YanKun Peng et al, 2007). In recent years, with the improvement of residents' living standards, consumers have paid more and more attention to the internal quality of apples (HaiLiang Zhang et al, 2009).

The traditional soluble solids content measurement method is destructive detection (WenChuan Guo et al, 2015), which not only causes the fruit to be unable to be reused, but also time-consuming and laborious, which makes difficult to meet the actual application requirements.

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Visible / Near Infrared spectroscopy can realize nondestructive and rapid measurement of physical and chemical information of samples (Gabrieli Alves de Oliveira et al, 2014; Agus Arip Munawar et al, 2019), and is widely used in the field of fruit quality detection (HuiJun Liu et al, 2015; ZhuanWei Wang et al, 2018; BartM Nicolai et al, 2014). For the study of nondestructive testing of apple soluble solids content, YanDe Liu et al (2007) used near-infrared spectroscopy to study the influence of different sampling distances on apple spectrum measurement; XiaoBo Zou et al (2007) used Fourier near-infrared spectroscopy to model and analyse apple soluble solids, and found that using iPLS and genetic algorithm together for characteristic wavelength screening can further improve the accuracy of the prediction model; JieWen Zhao et al (2005) and the like used principal component regression (PCR) and partial least squares (PLS) method to analyse apple soluble solids content. The research results show that the PLS model is more suitable for predicting the soluble solids content of apples than the PCR model; R Beghi et al (2012) carried out the measurement of soluble solids content of different apple varieties in the orchard environment based on the near-infrared spectroscopy technology, and achieved good accuracy. However, the detection system used is complicated and inconvenient to carry. The above-mentioned apple soluble solids content detection research focuses on methodological research. Although certain research progress has been made in equipment research and development, there is a lack of a complete solution from soluble solids content detection methods to system applications, which reduces its practical application value. Although there is portable detection equipment developed by scientific research institutes (Biao Yang et al, 2019; Xinyang Yu et al, 2016; Bin Wang et al, 2017), most of the equipment adopts the traditional black-and-white calibration method, and the dark reference spectrum and white reference spectrum are only collected once. In long-term use, the spectral intensity drift caused by the aging of the light source will affect the stability of the spectrum, resulting in the decline of the prediction accuracy of the equipment without self-calibration function.

This research intends to develop a portable apple soluble solids content detector based on visible / near-infrared spectroscopy, and realize the self-calibration function of the equipment by collecting the dark reference spectrum and white reference spectrum of apple samples in real time. It can communicate with the computer and mobile APP through the network port, Bluetooth, etc., to realize the portable detection of apple soluble solids content. The detector uses the visible / near infrared spectrum data of the apple sample to build the apple soluble solids content prediction model based on PLS, and compares different spectral predictions quantitatively. The influence of processing algorithm on full-band modelling and characteristic wavelength screening can realize the accurate detection of apple soluble solids content, hoping to provide a reference for fruit soluble solids content detection.

MATERIALS AND METHODS

DETECTOR DESIGN

Working Principle of Detector

The schematic diagram of the portable apple soluble solids content detector system is shown in Fig. 1.

The detector consists of an optical fibre probe, a point light source, an optical fibre loop, a microcontroller, an auxiliary circuit, a miniature spectrometer and a display interface. The light path switcher controls the opening and closing of the light path through the electromagnetic valve to realize the on and off control of the light path. The transmitting fibre 1 and the receiving fibre are both a one-to-two fibre. The receiving end of one receiving fibre directly receives the light information of the light source. The white reference spectrum is collected when the solenoid valve is opened, the dark reference spectrum is collected when the solenoid valve is closed, and the other is receiving fibre. The end receives the spectral information of the sample. When collecting the sample spectrum, the optical path switcher opens the light path between the emission fibre 1 and the emission fibre 2.

The light generated by the light source is uniformly irradiated on the surface of the apple through the ring fibre, and the light reflected by the apple surface enters the miniature spectrometer through the receiving fibre. In the soluble solids content prediction model modelling stage, the detector can receive commands from different terminals through external triggers, resistance screens, network ports, and Bluetooth modules, and perform spectral data collection and storage, and display the collected data in real time on the host computer and the resistance screen.

In the soluble solids content prediction stage, the microcontroller performs apple soluble solids content prediction based on the real-time collected spectrum data and the constructed prediction model and feeds the results back to the mobile phone APP interface and LCD screen.

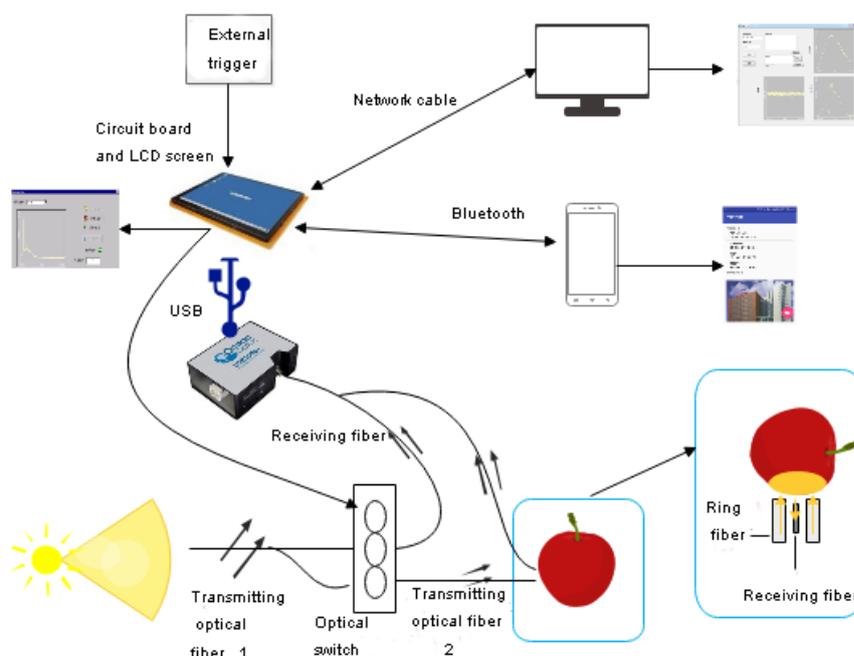


Fig. 1 - System schematic diagram

The physical map of the portable apple soluble solids content detector is shown in Fig. 2. The optical fibre probe has a ring optical fibre and an external trigger switch. The optical fibre loop includes a transmitting optical fibre 2 that conducts the light path of the light source and a receiving optical fibre that receives the reflected light information of the sample. The transmitting optical fibre 2 is composed of a single optical fibre and a ring optical fibre. The light source, miniature spectrometer and control circuit are located in the detector housing, and the light source adopts 3900 halogen lamps (Illumination Technologies).

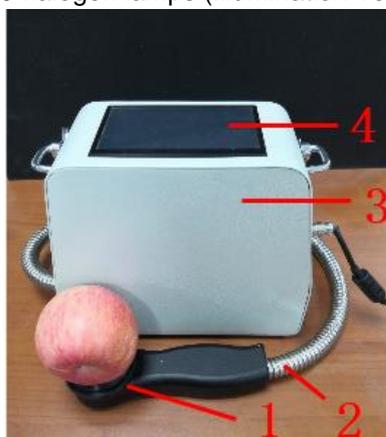


Fig. 2 - Portable detector of soluble solids content for apples

1) Optical fibre probe 2) Optical fibre loop 3) Detector housing 4) LCD resistive screen

Microcontroller and Related Circuit Design

The microcontroller of the soluble solids content detector uses a processor based on the ARM9 core, and WINCE is selected as the embedded operating system. The microcontroller directly controls the corresponding circuit through the IO port to complete the light path control, ensuring that the dark reference spectrum and the white reference spectrum for calibration can be collected at the same time when the sample spectrum data is collected. In addition, the detector also monitors the external trigger signal through IO. When the user presses a button, it can trigger a spectrum acquisition and soluble solids content measurement. The detector provides touch screen button operation for users to collect through the LCD resistive screen, which achieves the same function as the external buttons. The LCD resistive screen can display information such as spectral curves and sample soluble solids content. Because in the modelling stage of soluble solids content prediction model, the microcontroller needs to store a large amount of spectral data, therefore, an SD card is used to expand the storage space based on the FLASH storage that comes with the microcontroller.

The microcontroller can receive commands from different terminals. For example, using the TCP/IP protocol, the microcontroller can receive control commands from the host computer through the network port and send spectrum data to the host computer. In addition, the microcontroller can also be directly connected to the serial port Bluetooth module through the built-in RS232 serial port, which can ensure the small-range communication between the system and the mobile phone APP, thereby sending the predicted soluble solids content results to the mobile phone APP interface.

Miniature Spectrometer

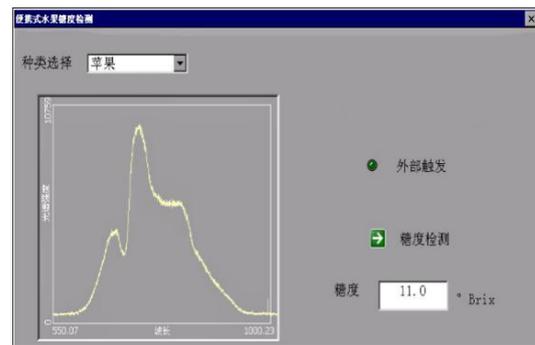
The detector uses a USB2000+ (Ocean Optics) miniature spectrometer with high signal-to-noise ratio for integrated development. The wavelength range of this spectrometer is 487-1147nm, and it has the advantages of small size, convenient installation and fixation. In addition, the miniature spectrometer has 16-bit A/D conversion resolution and 2048 wavelength points, and supports USB2.0 communication and RS232 communication. Call the USB2000+ library function in the WINCE system, and realize the parameter setting of the detector directly to the micro-spectrometer based on the USB protocol, and quickly obtain the real-time spectral data of the sample.

Software Design

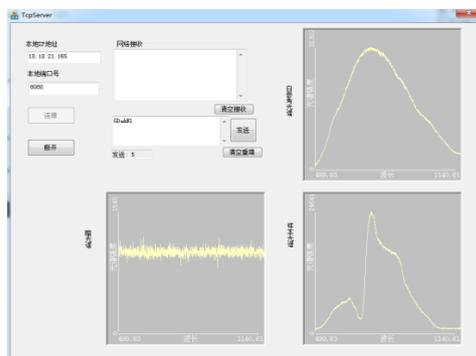
The software design of the detector includes WINCE system software, host computer software and mobile APP software design, so that the detector can be operated through different terminals to complete the collection, storage and real-time display of spectral data, as well as the construction of soluble solids content prediction model and the display of prediction results.



(A) Embedded system software interface



(B) The soluble solids content prediction interface of the embedded system



(C) Spectral data collection interface of host computer



(D) The mobile phone APP scans the Bluetooth device interface

Fig. 3 - Display interface of system software

The WINCE system software interface and the host computer software interface are realized by the Visual Studio platform based on C++ language programming. The WINCE system software spectrum data collection interface includes functions such as parameter setting, spectrum data collection, automatic storage, and real-time spectrum data display (Fig. 3a). Through the parameter setting function, the integration time of the spectrometer can be set; the spectral data collection can be realized through the external trigger and the soluble solids content detection button, and the spectral curve drawing and spectral data storage are automatically completed. The soluble solids content prediction interface (Fig. 3b) has user-operated touch buttons and a soluble solids content prediction result display box. The user only needs to press a button or an external trigger to complete the functions of spectral data collection, model prediction and soluble solids content display.

Because WINCE software is limited by the screen display space and flash storage space, this research further develops the host computer software (Fig. 3c). The host computer software is connected to the WINCE system software (referred to as the lower computer software) through the TCP/IP protocol. The host computer spectrum collection interface includes functions such as network port connection, spectrum collection control, spectrum curve display and automatic storage. The host computer software sends a spectrum acquisition instruction to the lower computer software, and the lower computer software automatically sends the collected dark reference spectrum, white reference spectrum and sample spectrum data to the host computer software after receiving the command. The host computer software automatically stores the collected spectrum data and displays it on the computer screen in real time. Through the displayed spectrum curve, it can be judged whether the collected signal of the spectrometer is saturated and whether the sample spectrum data is within the white reference spectrum data range.

The mobile app software (Fig. 3d) is programmed with JAVA language on the basis of Google's open source Android studio platform, which can realize the functions of device connection, soluble solids content detection and result display. The soluble solids content detection and display functions of APP software are similar to those of soluble solids content prediction interface (Fig. 3b), but not shown in Fig. 3d. The mobile app software is connected with the detector through Bluetooth, which can control the detector to collect spectral data and detect the sample soluble solids content. At the same time, the app software on the mobile phone can receive the sample soluble solids information fed back by the detector.

APPLE SOLUBLE SOLIDS CONTENT PREDICTION MODEL DESIGN

Experimental Materials

The apple samples used in the experiment were purchased from the Beijing Fruit Wholesale Market, and the variety was Yantai Fuji. A total of 160 apple samples with no obvious damage and scars were selected. In order to avoid influence of the external environment of the data, the skin cleaned apple fruit samples were placed in a laboratory environment 24 hours. Mark the equatorial position of each sample, and perform spectral data collection and soluble solids content measurement on the marked points. 120 samples were randomly selected to construct the model calibration data set, which was used to construct the apple soluble solids content prediction model, and the remaining 40 samples were used for model testing.

Spectrum Collection

Use the developed portable apple soluble solids content detector to collect sample spectrum data. After preheating the light source, spectral data collection is performed on the marked position of the apple sample. Experiments have found that when the integration time of the miniature spectrometer is set to 200ms, a strong sample spectrum signal can be obtained, and the white reference spectrum will not exceed the maximum value of the acquisition signal range. Collect the spectrum data three times on the same sampling point, and take the average value as the spectrum data of the sample. At the same time, obtain the corresponding white reference spectrum and dark reference spectrum at this time. Perform calibration according to formula (1) to obtain the corresponding spectral reflectance, so as to realize the spectrum collection and dynamic correction of the fruit sample by the detector.

$$reflectance = \frac{sample - dark}{white - dark} \quad (1)$$

In the formula, sample is the sample spectrum data, dark is the dark reference spectrum, and white is the white reference spectrum.

The spectrum measurement range of the USB2000+ mini spectrometer is 487-1147nm. Since the first and last bands of the spectrometer may contain large noise, in order to improve the prediction accuracy of the model, the detector selects the spectral data in the 550-900nm band for analysis.

Soluble Solids Content Measurement

Brix Apple sample measured using PAL-1 Brix detector (by ATAGO Co., LTD.'S., Tokyo, Japan) is obtained. In order to reduce the influence of storage time on the soluble solids content of the fruit, the soluble solids content of the apple sample is measured immediately after the end of the spectral data collection. For each apple sample, cut the pulp of 10mm thickness from the marked position and squeeze it to obtain the juice, drop the filtered juice onto the mirror surface of the refractometer, and record the soluble solids content displayed by the refractometer as the actual soluble solids content of the sample. Table 1 shows the statistical results of the soluble solids content of the calibration set and test set samples.

Table 1

Actual soluble solids content (°Brix) of apple's measured by the refractometer					
Sample set	Number of samples/pieces	Min/ °Brix	Max/ °Brix	Average/ °Brix	Standard deviation
Calibration set	120	10.1	16.6	13.15	1.21
Test set	40	10.2	16.3	13.22	1.25

SOLUBLE SOLIDS CONTENT PREDICTION MODEL

Model Construction

Partial least square (PLS) algorithm is widely used in spectral analysis because of its good stability and strong anti-interference ability (*Martin Andersson, 2009; Hong-Dong Li et al, 2018; Néstor F Pérez et al, 2009*). Therefore, the detector builds an apple soluble solids content prediction model based on the PLS algorithm. The optimal number of main factors of PLS algorithm is determined by the minimum root mean square error of cross validation (RMSECV). The original spectral data obtained by the spectrometer often contains random noise of the instrument. In addition, noise such as stray light will also affect the quality of the spectral data, which in turn affects the stability of the model. Therefore, this study quantitatively compared commonly used spectral data preprocessing algorithms, and determined the best preprocessing method by comparing the prediction accuracy of soluble solids content models based on different preprocessing methods. The preprocessing algorithms used in this study include: 9-point average smoothing (*XiaoLi Chu et al, 2004*), standard normal variate (SNV) (*R J Barnes et al, 1989*), maximum normalization (*RongQiang Gao et al, 2004*), 31-point first derivative method, and 51-point the second derivative method (*HaiLong Wang et al, 2015*).

Feature Wavelength Screening Algorithm

Since there is a large amount of redundant and collinearity information between the spectral variables, in order to avoid the complicated model and large amount of calculation caused by redundant spectral information (*YongHuan Yun et al, 2019*), it is necessary to screen the original spectral data by characteristic wavelengths, especially for the development of portable equipment, which can increase the speed of calculation and the efficiency of detection. At present, competitive adaptive reweighted sampling (CARS) and successive projections algorithm (SPA) (*JingZhu Wu et al, 2011; YanDe Liu et al, 2013; Chu Zhang et al, 2016; ShuXiang Fan et al, 2019; YunFei Xu et al, 2019*) are widely used in many feature wavelength screening methods, and have achieved good results in spectral data analysis. Therefore, this paper attempts to use these two algorithms to screen the characteristic wavelength of apple spectral data, so as to reduce the calculation amount of the model and further improve the prediction accuracy of the model. The CARS algorithm starts with the regression coefficient of the PLS model. The larger the absolute value of the regression coefficient, the more important the wavelength is. CARS is used to retain the wavelength variables with large absolute value of regression coefficient in PLS model, and remove the variables with small weight. A series of wavelength variable subsets are obtained through multiple screening, and each wavelength subset is verified interactively. According to the minimum root mean square error of cross validation, the best wavelength variable is obtained (*HongDong Li et al, 2009*). SPA uses the projection analysis of vectors to filter the variable combinations with the least redundant information among a large number of wavelength variables, so as to minimize the collinearity between variables, reduce the number of variables used in modelling, and improve modelling efficiency (*Mário César Ugulino Araújo et al, 2001; Wei Wang et al, 2019*).

Relevant literature shows that the direct use of SPA for characteristic wavelength screening will greatly reduce the number of characteristic wavelengths, but it will often reduce the prediction accuracy of the model. Therefore, the SPA algorithm is usually combined with other algorithms (Dan Liu et al, 2014).

Evaluation of Model Results

Correction correlation coefficient (Rc) and the predicted correlation coefficients (Rp) is a common indicator of the evaluation of the model quality. The larger the value of RC and RP, the better the prediction performance of the model. In addition, the RMSEC and RMSEP were used as the evaluation indexes of the model. The smaller RMSEC and RMSEP are and the closer they are, the better the prediction performance of the model is (ShuXiang Fan et al, 2015; ChengWen Chang et al, 2001).

RESULTS AND ANALYSIS

Full-Band Modelling Results Based on Different Preprocessing Algorithms

Table 2

PLS model results based on different preprocessing algorithms

Preprocessing methods	Number of main factors	RC	RMSEC / °Brix	RP	RMSEP / °Brix
None	11	0.889	0.552	0.862	0.692
Average smoothing	12	0.911	0.497	0.902	0.589
Maximum normalization	12	0.881	0.572	0.868	0.651
SNV	12	0.881	0.571	0.897	0.588
First derivative	12	0.921	0.468	0.876	0.611
Second derivative	13	0.909	0.502	0.856	0.689

The original spectrum data is preprocessed based on different preprocessing algorithms, and then the PLS algorithm is used to construct an apple soluble solids content prediction model based on the full-band spectral data. The results are shown in Table 2. Through quantitative comparative analysis, it is found that the prediction model of soluble solids content based on average smoothing pretreatment algorithm has the highest accuracy, with RC, RP, RMSEC and RMSEP of 0.911, 0.902, 0.497 ° Brix and 0.589 ° Brix, respectively. After average smoothing, the original reflectance spectral curves of 160 apple samples are shown in Fig. 4, and the prediction results of correction set and prediction set are shown in Fig. 5. Therefore, the subsequent analysis is based on the spectral data after average smoothing pretreatment.

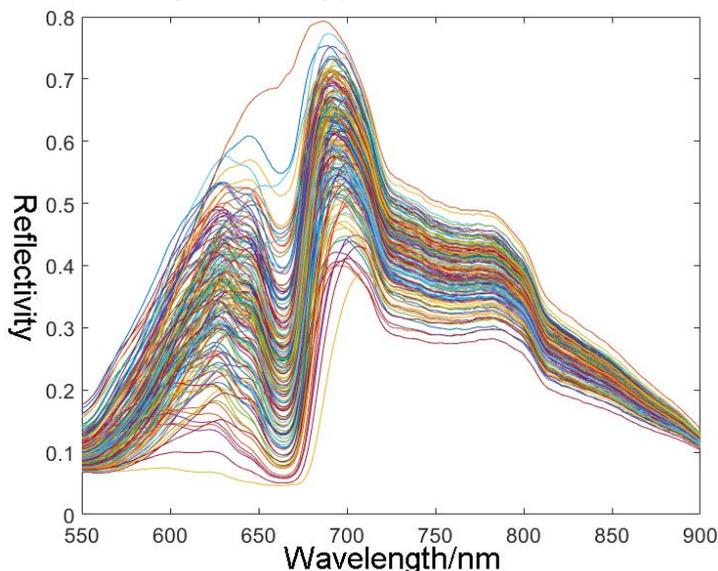


Fig. 4 - Reflectance curve of apple sample' s spectrum

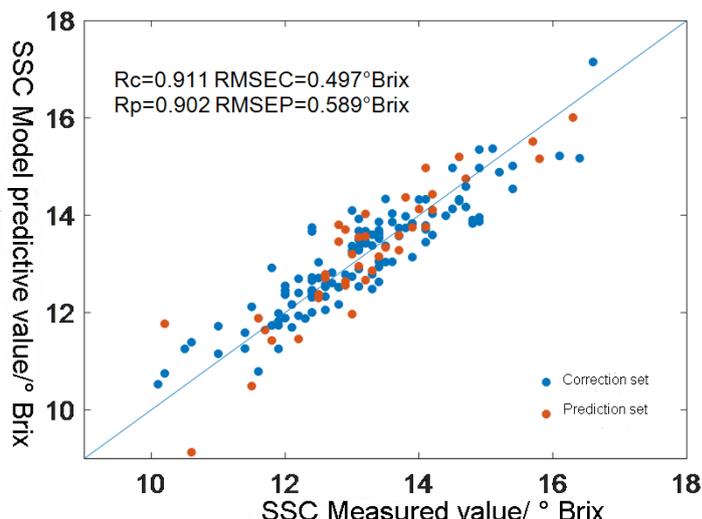


Fig. 5 - Prediction results of PLS model for apple' s SSC based on average smoothing preprocessing algorithm

Modelling Results Based on Characteristic Wavelengths

The CARS algorithm is used to screen the preprocessed spectral data with characteristic wavelengths, and the characteristic wavelengths with high correlation with the prediction of sample soluble solids content are selected. The results are shown in Fig. 6, as the number of sampling increases, the number of modelling variables gradually decreases, and RMSECV gradually decreases as the number of characteristic wavelengths decreases. When the sampling frequency is 47 times, the RMSECV reaches a minimum value of 0.492. In this case the model variables should be 57.

When the sampling times are further increased, the number of modelling variables continues to decrease, which leads to the elimination of characteristic wavelengths related to soluble solids content, resulting in the gradual increase of RMSECV. Therefore, the optimal number of modelling variables was determined by the minimum value of RMSECV, that is, 57 characteristic wavelengths were selected by CARS algorithm to build the prediction model of apple soluble solids content. Based on the selected 57 characteristic wavelengths, a PLS model was established to detect the soluble solids content of apple. The RC and RP were 0.937 and 0.906, RMSEC and RMSEP were 0.418 ° Brix and 0.545 ° Brix, respectively. Compared with the full band spectral analysis, the modelling wavelengths decreased from 1030 to 57, and the modelling results were slightly improved.

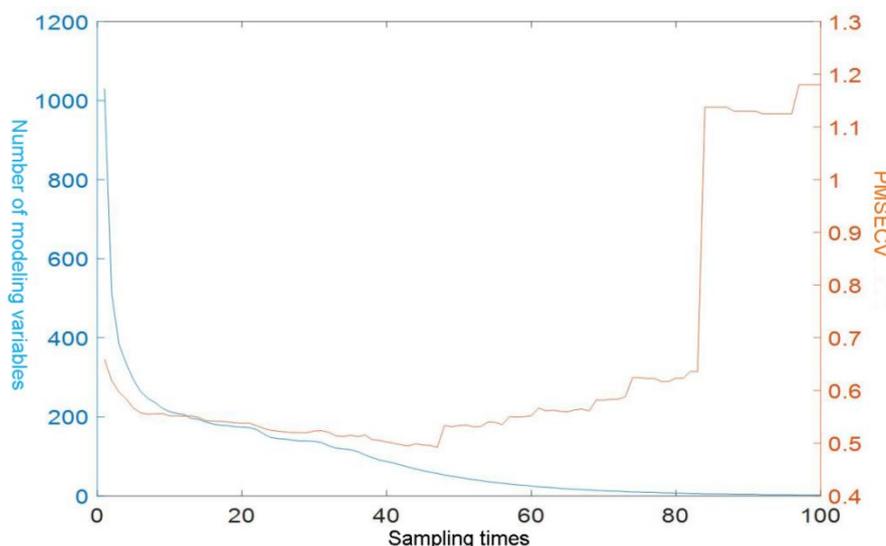


Fig. 6 - Effective wavelengths selected by CARS

For the real-time analysis of apple soluble solids content, the shorter the characteristic wavelength, the shorter the model prediction time. In order to further improve the prediction efficiency, on the basis of the CARS algorithm, the SPA algorithm is further used to optimize the characteristic wavelength.

Fig. 7 shows 17 characteristic wavelengths selected by SPA algorithm on the basis of 57 wavelengths selected by CARS.

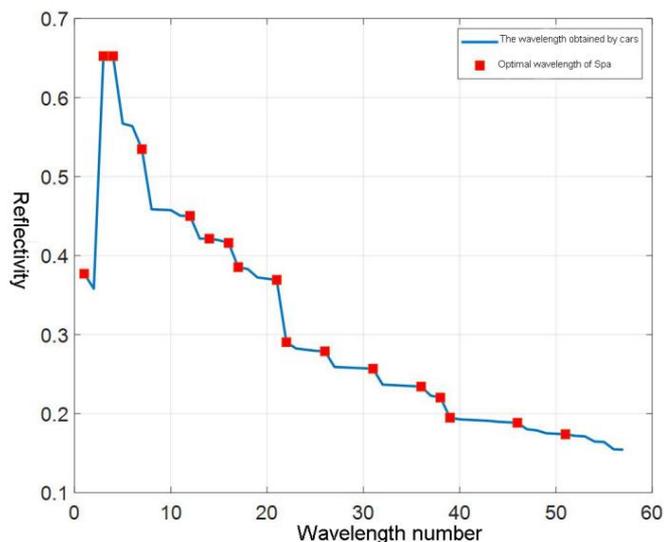


Fig. 7 - Effective wavelengths selected by CARS-SPA

The optimized prediction model of soluble solids content was constructed by using the selected 17 characteristic wavelengths. The test results are shown in Fig. 8.

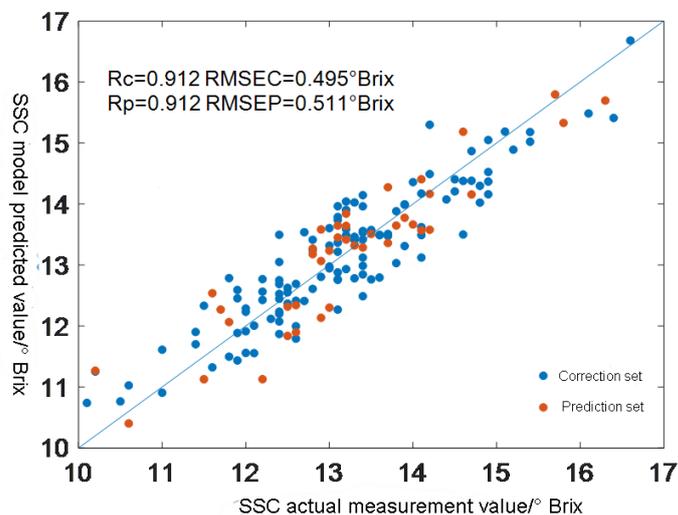


Fig. 8 - Measurement results versus prediction results of apple' s SSC using CARS-SPA simplified model

Compared with the prediction results based on the full band, the optimized soluble solids content prediction model not only reduced the number of variables, but also improved the prediction results.

Finally, 17 characteristic wavelengths for soluble solids content analysis were determined as follows: 637.52, 691.59, 696.45, 716.11, 739, 761.67, 782.1, 795.72, 801.01, 816.16, 821.73, 834.77, 847.41, 854.5, 865.74, 868.94, 876.59 nm.

According to the above 17 characteristic wavelengths, an optimized apple soluble solids content prediction model is established, as shown in formula (2).

$$\begin{aligned}
 Y = & -7.13X_{637.52} + 119.28X_{691.59} - 184.32X_{696.45} \\
 & + 249.23X_{716.11} - 357.54X_{739} + 260.47X_{761.67} \\
 & - 64.23X_{782.1} - 147.51X_{795.72} - 288.61X_{801.01} \\
 & + 228.28X_{816.16} + 174.87X_{821.73} + 338.89X_{834.77} \\
 & + 454.03X_{847.41} + 191.07X_{854.5} - 357.37X_{865.74} \\
 & - 411.16X_{868.94} - 430.68X_{876.59} + 37.97
 \end{aligned} \tag{2}$$

Among them, Y is the predicted soluble solids content of the apple sample, and X_{637.52}... X_{876.59} is the spectral reflectance corresponding to 17 wavelengths extracted by CARS-SPA algorithm. Integrate the optimized soluble solids content prediction model into the tester for fast and nondestructive testing of the soluble solids content of apples.

CONCLUSIONS

This research intends to develop a portable apple soluble solids content detector based on near-infrared spectroscopy technology, which can realize the rapid and accurate detection of apple soluble solids content. The main research conclusions are as follows.

(1) A portable apple soluble solids content detector is designed, which is mainly composed of optical fibre probe, optical fibre loop, micro spectrometer, microcontroller and display interface. It can communicate with computer terminal and mobile app through network port, Bluetooth and other ways to realize the portable detection of apple soluble solids content. By collecting the dark reference spectrum and white reference spectrum of apple samples, the self-calibration function of the device can be realized.

(2) 160 apple samples were used to construct the prediction model of apple soluble solids content, and the prediction accuracy of models based on different preprocessing methods was quantitatively compared. The results showed that the accurate prediction of apple soluble solids content could be achieved by using average smoothing to preprocess spectral data and establishing PLS model. The RC, RP, RMSEC and RMSEP were 0.911, 0.902, 0.497 ° Brix and 0.589 ° Brix, respectively. Based on the selected 17 characteristic wavelengths, the accuracy of soluble solids content prediction model was further improved. The RC, RP, RMSEC and RMSEP were 0.912, 0.912, 0.495 ° Brix and 0.511 ° Brix, respectively.

The portable apple soluble solids content detector developed in this study realizes the rapid and nondestructive detection of apple soluble solids content, and its application scope can be further extended to the soluble solids content detection of pear, thin skin watermelon, tomato and other spherical fruits, so as to provide support for the rapid detection of fruit soluble solids content.

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