A Study to Detect the Soluble Solid Content and pH for Bingtang Orange Non-destructively using Near Infrared Spectroscopy

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Abstract **– We study the potential of near infrared spectroscopy (NIRS) in the wavelength range of 350-1800 nm to determine the soluble solid content and pH for Bingtang orange. Partial least square (PLS), principal component regression (PCR) and multiple linear regression (MLR) techniques were carried out. PLS model was found to be the best for prediction based on treating the spectra dates with first-order differential technique. The multiple correlation coefficients for calibration were found to be 0.9360 for SSC and 0.8432 for pH, respectively. The correlation coefficients for prediction were found to be 0.7950 for SSC and 0.8196 for pH, respectively. The results indicated that NIRS could be used to predict internal quality of Bingtang orange non-destructively.**

Keywords - Bingtang orange; Soluble solid content; pH; Near infrared reflectance spectroscopy

I. INTRODUCTION

Orange is recognized as an important agriculture product in China and Bingtang orange is one of the most favorite among various kinds of orange [1]. Enterprise and consumer preference and price highly on varies qualities of oranges. Thus, there is a need for reliable technique to evaluate the qualities of orange.

Over the last few decades, quality evaluation of agriculture products has been a main focus for researchers. The internal quality of fruits is varied, such as soluble solids content (SSC), sweetness, acidity, fibers, pH, and so on. Traditionally, the methods for determining the taste of fruits and vegetables are destructive and unusable. Therefore, non-destructive testing techniques for the internal quality have gained momentum. Near infrared spectroscopy (NIRS) is an important technique amongst various non-destructive methods for determination of fruits and vegetables. Many detecting techniques have been proposed by using NIRS. Different kinds of fruit have been determined using NIRS, such as peach, apricot, apple, orange and so on [2-5]. The reports on determination of fruits based on NIRS were concern about various characters, including total suspended solids (TSS), hardness, firmness, acidity and others [6-8].

With the help of NIRS, a detection technique of SSC and pH for Bingtang orange is proposed in this paper. In practice, however, the components of samples are complex, and the near infrared spectrum dates original cannot be used directly because of the impacts of noise. In order to reduce the influence of noise, 9 point moving average window smoothing, first-order differential and multiplicative scatter correction are used for the Bingtang orange spectral pretreatment, then the predictive model is set up by partial least square (PLS), principal components regression (PCR) and multivariable linear regression (MLR), moreover, the accuracy is compared.

This paper is organized as follows. The materials and methods are presented in section 2. The predicted results and discussions are given in section 3 and a brief conclusion is included in section 4.

II. MATERIALS AND METHODS

Orange samples:Fresh orange were procured from local fruit market. The samples were brought to laboratory and screened manually to discard the scarred and scratched ones. Sizeable oranges were wiped to remove dirt and kept for 10 days at 20°C and 60% RH. Then, the samples were randomly divided into different groups with thirty samples in calibration set and fifteen samples in prediction set, moreover, five samples were used as spare ones.

NIR Spectra acquisition: Transmittance spectra in wavelength 350-1800 nm of samples, were acquired using a NIR-spectrometer (model QualitySpec Pro, 1 nm resolution ASD Inc., USA). Then, the transmittance spectra of samples were acquired three times independent at an interval of 1 nm for the wavelength range of 350-1800 nm.

Determination of SSC and pH: Immediately after recording the spectra, juice of the whole orange at ambient room temperature. Juice was filtered through a new piece of muslin cloth every time. The SSC of the filtered juice was measured thrice using a refractive saccharimeter (model PR-101 α, range 0.0-45% Brix, least count 0.1% Brix, Japan) and pH was determined using a digital pH meter (model Testo230, range 0.0-14.0 pH, accuracy 0.01 pH, Germany). Then, mean values were used for NIR calibration and prediction.

NIR spectral data were processed with Unscambler 9.5 software and Matlab 7.0 software. In order to reduce the influence of random errors, the spectral date was pretreated with 9 point moving average window smoothing, first-order differential and multiplicative scatter correction, respectively. Typical spectral data of oranges used for the calibration and prediction of SSC and pH were plotted to analysis the feature of the spectra.

In order to develop the NIR model for predicting SSC and pH of oranges non-destructively, three models were performed, including partial least square regression (PLS), principal components regression (PCR) and multiple linear regression (MLR). Some parameters such as the multiple correlations coefficients (R), the root mean square error of calibration (RMSEC) and the root mean square error of prediction (RMSEP), were selected to evaluate the models.

III. RESULTS AND DISCUSSION

Typical spectral curves in the wavelength of 350-1800 nm for the samples are presented in Fig 1. The peaks and depressions in spectra show the transmittance characteristics of Bingtang orange. Within the range of the study, each one has its own relative values in the region of spectra.

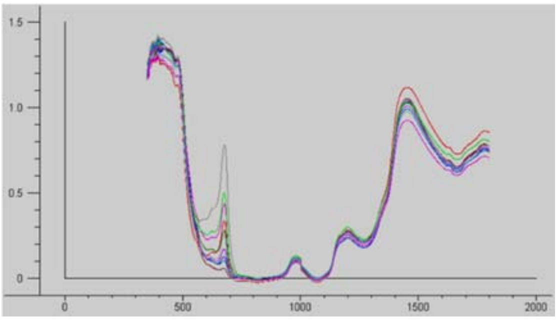


Fig.1 Typical NIR spectra of samples in wavelength of 350-1800 nm

When using PLS model, the effect of calibration accuracy with various pretreatment methods is showed in Table 1. R value and RMSEC value for calibration and validation of SSC in first-order differential pretreatment were found to be 0.9360 and 0.4520, respectively. R value in first-order differential is higher than the other two methods, and RMSEC value is the lowest of them. There is a small difference in R values for calibration of pH between first-order differential and multiplicative scatter correction, which were 0.8432 and 0.8474, respectively. RMSEC value is lower when first-order differential pretreatment is used. Therefore, first-order differential performed the best of three pretreatment methods.

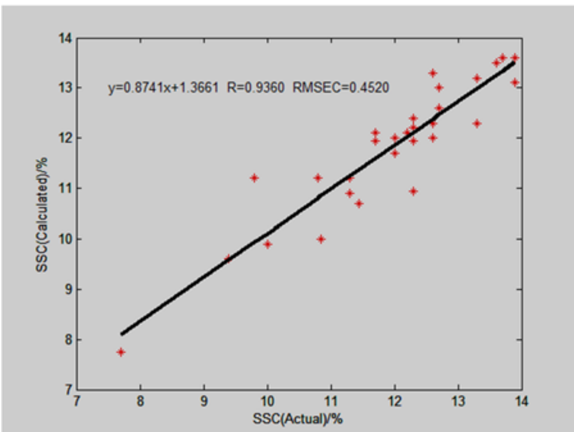
TABLE 1. EFFECT OF VARIOUS PRETREATMENT METHODS IN PLS MODEL FOR CALIBRATION OF SSC AND PH

Index	Pretreatment Method	Principal Factor	R	RMSEC
SSC	9 point moving average window smoothing	6	0.8724	0.7261
	first-order differential	6	0.9360	0.4520
	multiplicative scatter correction	6	0.8235	0.6542
pH	9 point moving average window smoothing	6	0.8211	0.3623
	first-order differential	7	0.8432	0.1400
	multiplicative scatter correction	7	0.8474	0.3427

The accuracy of various methods such as PLS, PCR and MLR models, is compared based on the first-order differential pretreatment. The results (Table 2) show that PLS model performed better among three models. R value and RMSEC value for PLS model were found to be 0.9360 and 0.4520 respectively during the SSC calibration. The higher R and lower RMSEC in PLS model indicate that the calibration of SSC is much better and stable. Further, the least square method has been applied to get the linear curve fitting and the slope is approximately 45° (Fig. 2). The same situation exists in the pH calibration.

TABLE 2. R, RMSEC OFPLS, PCR AND MLR MODELS FOR CALIBRATION OF SSC AND PH

Index	Model	R	RMSEC
SSC	PLS	0.9360	0.4520
	PCR	0.8421	0.6812
	MLR	0.8984	0.5426
pH	PLS	0.8432	0.1400
	PCR	0.7538	0.1618
	MLR	0.8398	0.1406



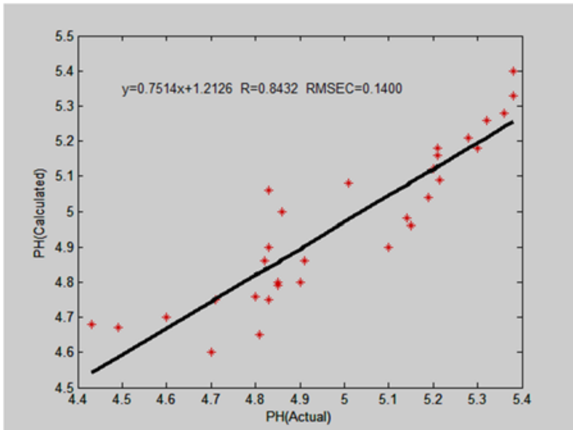


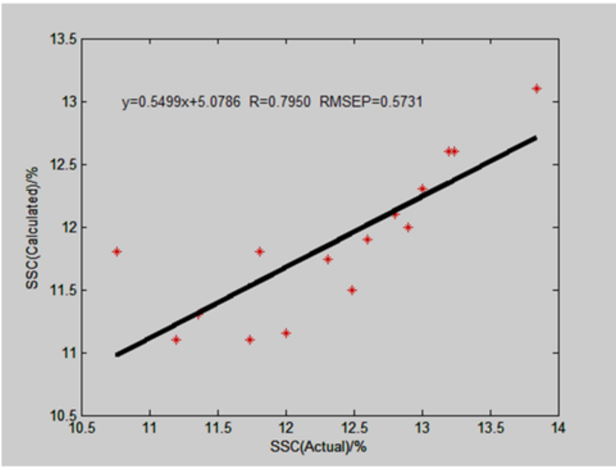
Fig.2 Calibration results of SSC and pH using PLS model.

In order to compare the stability and reliability of different models, samples in prediction set were tested by some models including PLS, PCR and MLR. The accuracy of various models is compared and the results proved that PLS model is better than the two other models (Table 3). In the prediction results of SSC and pH, R value in PLS model were found to be the highest and RMSEP value were found to be the lowest. Scatter plots drawn from PLS model show that the slope of the curve is near to 45°, thus indicate the predicted values may be near to the measured ones (Fig. 3).

TABLE 3. R, RMSEP OF PLS, PCR AND MLR MODELS FOR PREDICTION OF SAMPLES

Index	Model	R	RMSEP
SSC	PLS	0.7950	0.5731
	PCR	0.7437	0.7657
	MLR	0.7681	0.5831
pH	PLS	0.8196	0.1353
	PCR	0.7632	0.1618
	MLR	0.7622	0.1417

DOI 10.5013/IJSSST.a.17.49.05 ISSN: 1473-804x online, 1473-8031 print



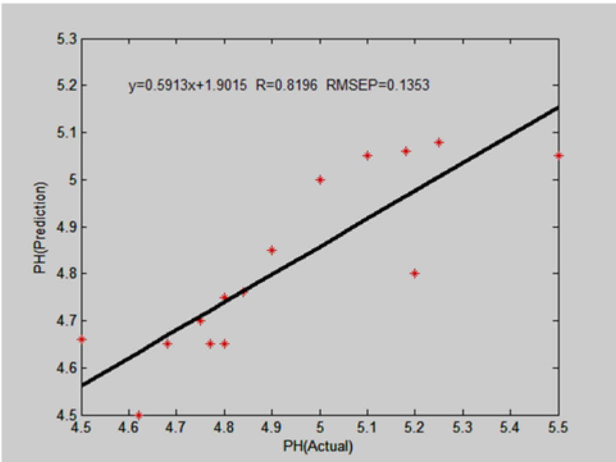


Fig.3 Prediction results of SSC and pH using PLS model.

IV. CONCLUSION

In this paper, 9 point moving average window smoothing, first-order differential and multiplicative scatter correction are used for the spectral pretreatment of Bingtang orange, then the predictive model is set up by partial least square (PLS), principal components regression (PCR) and multivariable linear regression (MLR). Moreover, the accuracy of various models is compared. The results show that PLS model based on first-order differential pretreatment display the higher R value and lower RMSEC/RMSEP value. Therefore, the prediction of SSC and pH of Bingtang orange using PLS model based on first-order differential pretreatment is much more reliable and stable.

FUNDING

Project supported by the Research Foundation of Education Department of Hunan Province, China (15C1092) and the Research Foundation of Key Laboratory of Intelligent Control of Ecological Agriculture in Wuling Mountain Area, China (ZNKZ2015-3).

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