NEAR INFRARED DIFFUSE REFLECTANCE MEASUREMENT SET-UP IN NON-DESTRUCTIVE BRIX MEASUREMENT FOR INTACT PINEAPPLES

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To my beloved parents, thank you.

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ABSTRACT

Conventional Brix prediction of pineapple is time-consuming and destructively. Even few of the applications of near infrared spectroscopy in diffuse reflection mode had been implemented in determining the Brix of pineapple, those applications did not investigate the effect of pineapple surface (geometrical effect) and the measurement setup on the prediction performance. This study investigates the geometrical effect with three parameters including the effect of different parts of pineapple on the diffuse reflectance, relationship between diffuse reflectance and soluble solids content (SSC), and effect of measurement position on the calibration model. The measurement setup was investigated through pre- and post-dispersive (with fiber optic design) NIRS technique. Three parameters were studied with pre-dispersive sensor. First, the effect of acquired difference reflectance from different parts of pineapple i.e. top, middle, and bottom was investigated with boxplot technique. Then, the relationship between the diffuse reflectance and SSC was evaluated with correlation plot. Lastly, nine independent artificial neural networks were separately trained to investigate the geometrical effects on different parts of pineapple. Results show that the concave surface of top and bottom parts of pineapples would affect the reflectance of light and deteriorate the prediction performance. With bifurcated fiber optic design, the predictive model of middle part of pineapples achieved the best performance i.e. root mean square error of prediction and correlation coefficient of prediction of 1.313 °Brix and 0.7408 respectively. The main finding of the research is that the geometrical effect that affects the Brix prediction can be minimized by proper measurement setup.

ABSTRAK

Ramalan nanas Brix konvensional memakan masa dan merosakkan. Walaupun beberapa aplikasi spektroskopi inframerah dekat dalam mod refleksi difus telah dilaksanakan dalam menentukan Brix nanas, aplikasi tersebut tidak menyelidiki pengaruh permukaan nanas (efek geometri) dan pengaturan pengukuran pada prestasi ramalan. Kajian ini mengkaji kesan geometri dengan tiga parameter termasuk pengaruh bahagian nanas yang berlainan pada pantulan resapan, hubungan antara pantulan meresap dan kandungan pepejal larut (SSC), dan pengaruh kedudukan pengukuran pada model penentukuran. Penyediaan pengukuran disiasat melalui teknik NIRS sebelum dan sesudah penyebaran (dengan reka bentuk gentian optik). Tiga parameter dikaji dengan sensor pra-penyebaran. Pertama, kesan pemerolehan perbezaan yang diperoleh dari bahagian nanas yang berbeza iaitu bahagian atas, tengah, dan bawah disiasat dengan teknik boxplot. Kemudian, hubungan antara pantulan difus dan SSC dinilai dengan plot korelasi. Terakhir, sembilan rangkaian saraf tiruan bebas dilatih secara berasingan untuk mengkaji kesan geometri pada bahagian nanas yang berlainan. Hasil kajian menunjukkan bahawa permukaan cekung bahagian atas dan bawah nanas akan mempengaruhi pantulan cahaya dan merosakkan prestasi ramalan. Dengan reka bentuk serat optik bifurcated, model ramalan bahagian tengah nanas mencapai prestasi terbaik, iaitu ralat punca min punca ramalan dan pekali korelasi ramalan masing-masing 1.313°Brix dan 0.7408. Penemuan utama penyelidikan adalah bahawa kesan geometri yang mempengaruhi ramalan Brix dapat dikurangkan dengan penyusunan pengukuran yang betul.

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dispersive sensor i.e. calibrated diffuse reflectance, calibrated diffuse reflectance with normalization, and calibrated diffuse reflectance with standard normal variate (SNV).

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LIST OF SYMBOLS AND ABBREVIATIONS

SSC	–	Soluble Solids Content
NIR	–	Near Infrared
NIRS	–	Near Infrared Spectroscopy
LED	–	Light Emitting Diode
ANN	–	Artificial Neural Network
SNV	–	Simple Normal Variate
LM	–	Levenberg-Marquardt
C	–	Carbon
O	–	Oxygen
N	–	Nitrogen
H	–	Hydrogen
EH	–	Emission Head
IS	–	Integrating Sphere
fNIRS	–	Functional Near Infrared Spectroscopy
MLR	–	Multiple Linear Regression
PCR	–	Principle Component Regression
PLS	–	Partial Least Squares
LVs	–	Latent Variables
BR	–	Bayesian Regularization
SCG	–	Scaled Conjugate Gradient
KS	–	Kennard-Stone Algorithms
SEC	–	Standard Error of Calibration
RMSEP	–	Root Mean Square Error of Prediction
RMSEC	–	Root Mean Square Error of Calibration
Rp	–	Correlation Coefficient of Prediction
Rc	–	Correlation Coefficient of Calibration

n	–	Number of Samples
SSC_{actual}	–	Measured Soluble Solids Content
$SSC_{predicted}$	–	Predicted Soluble Solids Content
I_c	–	Calibrated Diffuse Reflectance
I_{LED}	–	Raw Data
I_d	–	Dark Reference Value
I_w	–	White Reference Value
I_N	–	Intensity of Calibrated Diffuse Reflectance with Normalization
I_{Total}	–	Total Calibrated Diffuse Reflectance
I_{SNV}	–	Intensity of Calibrated Diffuse Reflectance with SNV
σ_{LED}	–	Standard Deviation of Calibrated Diffuse Reflectance
$\bar{x}_{LED}$	–	Mean of Calibrated Diffuse Reflectance

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CHAPTER 1

INTRODUCTION

1.1 Background of the study

Pineapple is a kind of popular fruit in tropical which is well-received by the society. It contributes over 20% of the tropical fruit produced in the world. Besides, pineapple contains vitamin C, vitamin A and fiber and has many health benefits. In Malaysia, export pineapple product can be categorized into four major types including pineapple juice, canned pineapple, fresh pineapple, and ornamental. According to the information of Malaysia Pineapple Industry Board (MPIB), the total exportation of pineapple product reached RM184 million in 2018 [9]. Malaysia pineapple has become a new source of wealth for the country. Among the internal quality of pineapple, the soluble solids content (SSC) with unit °Brix is used as the internal quality indicator of pineapple [10]. The SSC is one of the main factors that affect its market value and quality [11]. However, the conventional Brix measurement of pineapple is destructively and time-consuming [12]. Firstly, the pineapple was dissected and the pulp was squeezed into juices. Then, the juice was measured with digital refractometer to get its Brix. The invasive and time-consuming process is impossible to ensure that each exported pineapple product able to fulfil the exported Brix requirement.

Near infrared (NIR) region is a part of electromagnetic radiation with spectral range from 780 to 2500nm [13]. NIR energy with specific wavelength can be partially absorbed by specific molecular bonds that consist of hydrogen e.g. C-H and O-H to become mechanical energy of molecular overtone and vibrations [14]. The amount of this energy transformation (also known as absorption) is affected by the chemical composition and the physical properties of an examined sample. By using calibration or machine learning methods, the hidden information of the acquired NIR spectra can be extracted and utilized to quantitatively or qualitatively analyze the samples [15]–[18].

Near infrared spectroscopy (NIRS), a rapid and non-invasive sensing technique in qualitative and quantitative analysis using NIR region, has been widely implemented in various fields e.g. construction [19], agriculture [20]–[29], medical [30]–[32], drug [33]–[35], tobacco [36], [37], wood species [38]–[40], textiles [41],[42], and soil [43]–[48]. NIRS is promising to be an alternative of various existing sensing techniques which is destructive, time-consuming, and expensive. A typical NIRS data acquisition consists of five main steps. First, the positions of the energy source, the NIR detector, and the measured object are fixed in a NIR acquisition system. Second, white and dark calibrations are conducted by correcting the measured NIR spectrum with respect to the 100% and 0% reference spectra. After the signal calibration, an examined sample is allocated at the position of the measured object for NIR spectrum acquisition. In most cases, the acquired spectrum is pre-processed to reduce or remove unwanted signals e.g. baseline shifts due to scattering effects. Finally, the relationship between the pre-processed spectrum to the components of interest is established using machine learning or chemometrics. This is because the information of NIR spectrum is highly overlapping and corelated to its adjacent wavelengths.

Each sample has a different exterior appearance and composition. According to the Beer-Lambert law, the light absorbance is linearly proportional to the concentration of absorbing composition for non-scattering samples under constant light path arrangement [49]–[51]. However, this law is inapplicable for scattering samples due to the variable of individual photon and the complication of light scattering in the samples [52]. In a scattering sample, the detected light from the sample will change according to the appearance and dimension of each sample. This implies that the positioning of NIRS light illumination and detection (i.e. a suitable sensing mode) will affect the performance of NIRS in terms of the quality and robustness of the acquired data.

In general, NIRS has been classified into three basic acquisition modes i.e. reflection, transmission, and interaction collecting in the NIR energy from samples [1]. These sensing modes can be discriminated according to the positions of energy source and detector. For the reflection, the energy source and detector are always mounted in ways i.e. angle between the source and detector is 45˚[29], [43], [53] that specular reflectance will be eliminated [54]. For the transmission, the energy source is placed opposite of the detector. For the interaction, the light source and detector are positioned parallel to each other by assuming that the detector will not acquire any specular reflectance and diffuse reflectance of the surface. In short, both the reflection and interaction aim to acquire diffuse reflectance and avoid specular reflectance.

When the light reflects from a surface is scattered in many angles in case of only the specular reflectance, it is called diffuse reflectance. Near infrared diffuse reflection mode has revealed its potential as a powerful and non-destructive technique for rapid analysis [49]–[57]. Despite abundant studies of diffuse reflection were carried out in non-destructive Brix determination, lack of studies was concerned about the underlying mechanism. This could limit the understanding of diffuse reflection mechanism and underestimate its potential.

Optical geometry can be defined by the position between the source and detector and the sample's surface [52]. Most of the studies were using the fiber optic reflectance probe and integrating sphere module for diffuse reflectance acquisition [63]–[70]. Basically, the fiber optic reflectance probe will directly apply either contact or contactless measurement without considering the effect of the sensor position [71],[72]. The typical design of the fiber optic probe is the several light source cables and detection cable are always mounted together in a single coaxial cable [4]. Due to the aforementioned design, the fiber optic reflectance probe is always 0˚ angle toward the sample in any position.

Consequently, the diffuse reflectance due to the geometry of sample has not been substantially studied. The uneven skin of sample may have unexpected reflection which is worthy to further investigate. Thus, a better understanding about the diffuse reflection is needed to improve the accuracy of acquired signals. Better understanding will definitely improve the accuracy of non-destructive internal quality measurement using NIRS technology. This is because better understanding of diffuse reflection will lead to a better diffuse reflectance acquisition design which will have a better signal to noise ratio (SNR). A higher accuracy of internal quality prediction will ultimately help the farmer in harvesting and reduce the unnecessary fruit waste and indirectly improve the global fruit security.

1.2 Problem statement

Currently, conventional Brix measurement for pineapple is destructively and time-consuming. Near infrared spectroscopy (NIRS) is a promising tool in rapid, fast, and non-destructive Brix measurement of fruit [2]. Even though few of the applications of NIRS in diffuse reflection mode had been implemented in determining the internal quality of pineapple, those applications did not investigate the effect of pineapple surface (geometrical effect) and the measurement setup (pre- and post-dispersive technique) on the prediction performance. Lack of the understanding about the geometrical effect and measurement setup on the diffuse reflectance acquired from the pineapple will deteriorate the performance of NIRS.

Furthermore, the uneven skin on top, middle, and bottom of the pineapple may provide different and unexpected reflection which will affect the internal quality prediction. Thus, the geometrical effect on pineapple and measurement setup of diffuse reflection mode for pineapple internal quality prediction non-invasively is worth to be further studied. The Brix of pineapple will remain the same once they are harvested [10]. Better understanding in diffuse reflection will help the farmer in harvesting and reduce the unnecessary fruit waste and then improve the global fruit security.

1.3 Hypothesis

A better understanding of pre- and post-dispersive NIRS measurement setup can improve the Brix prediction performance for pineapple.

1.4 Aim

The aim of the research is to provide a better understanding of pre- and post-dispersive NIRS measurement setup in diffuse reflection mode to improve the Brix prediction performance for intact pineapple.

1.5 Objectives

This research work embarks on the following objectives:

1. To study the parameters that involve in validating the consistency and correctness of pre-dispersive near infrared (NIR) diffuse reflectance acquisition for non-destructive Brix determination of intact pineapple.
2. To establish the relationship between the acquired pre-dispersive NIR diffuse reflectance and the Brix of intact pineapple using the optimal parameters.
3. To compare the accuracy of pre-dispersive and post-dispersive NIR diffuse reflectance acquisition in non-destructive Brix determination of intact pineapple.

1.6 Scopes of study

The scope of this research is stated as below:

1. This research is only focused on two effects on the diffuse reflection mode:
    - Measurement setup i.e. pre- and post-dispersive techniques of near infrared spectroscopy.
    - Geometrical effect of intact pineapple including the top, middle, and bottom parts.
2. Two existing near infrared sensors with pre- and post- dispersive technique were utilized in data acquisition：
    - The pre-dispersive sensor consisted of photodiode and five light emitting diodes with five different wavelengths i.e. 780, 851, 870, 910 and 940nm.
    - The post-dispersive sensor consisted of bifurcated fiber optic design and a spectral sensor which able to detect wavelengths range at 680, 730, 760, 810 and 860nm.
3. Three parameters were investigated in this study:
    - Effect of different parts of pineapples i.e. top, middle, and bottom on the acquired diffuse reflectance.

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APPENDIX A

LIST OF PUBLICATIONS

1. F. W. Hong, and K. S. Chia, "A review on recent near infrared spectroscopic measurement setups and their challenges," *Measurement*, vol. 171, p. 108732, 2021. (ISI indexed, Q1, impact factor: 3.364)
2. F. W. Hong, and K. S. Chia, "Investigation of parameters that affect the acquired near infrared diffuse reflected signals in non-destructive soluble solids content prediction" *Engineering Journal,* vol. 24, no. 6, p. 79-90 2020. (Scopus indexed)
3. F. W. Hong, and K. S. Chia, "Design and Develop a Near-Infrared System for Intact Pineapples" *MALTESAS*, vol. 1, no. 2, p. 12-23, 2018. (Google Indexed)