การใช้ Near-Infrared spectroscopy เพื่อทำนายคุณลักษณะของข้าวเปลือก

Development of calibrations for paddy rice using near-infrared spectroscopy

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Abstract

Near-infrared (NIR) spectroscopy provides an alternative, nondestructive technology for measuring constituents of biological materials. Multivariate calibration models are often used incombination with NIR spectroscopic techniques to predict physical or chemical sample properties. The aim of this study is to develop robust calibration models to predict protein and moisture contents in paddy. In this study 33 paddy samples were measured for protein and moisture contents at 4 ºC and at room temperature (25-27 ºC) over on extended wavelength range from 730-1,100 nm by AG-RD spectrometer at 0.5 nm intervals. Calibrations were developed using Unscrambler 9.8 Software (CAMO Software Japan Co. Ltd) for all samples. Initial calibrations for both moisture and protein content were relatively good (SECV= 0.77, R^2=0.96 and SECV = 0.43, R^2=0.77, respectively), considering that spectra were taken through husk. There are no stratification for both temperature conditions and for moisture content (SECV= 0.89 and R^2=0.93 for cool and SECV = 0.77 and R^2=0.96 at room temperature), while those for protein content were SECV = 0.47 and R^2=0.70 for cool samples and SECV= 0.42 and R^2=0.62 for room samples. Wavelength selection was then executed in an effort to improve calibration performance and results showed small improvement with R^2 values but the general situation remained the same with protein calibrations having R^2 of 0.83 and SECV of 0.35 and moisture calibrations having R^2 of 0.94 and SECV of 0.94. In order to develop robust calibrations various pretreatment methods should be executed do determine the best results.

Keywords: Near infrared spectroscopy, moisture, protein, paddy

บทคัดย่อ

Near-Infrared (NIR) spectroscopy เป็นวิธีการหนึ่งที่สามารถใช้วัดองค์ประกอบของวัสดุทางชีวภาพได้ การใช้คลื่นแสง NIR ร่วมกับสมการหลายตัวแปรสามารถทำนายลักษณะทางเคมีและชีวภาพของตัวอย่างวัสดุได้ วัตถุประสงค์ของงานวิจัยนี้เพื่อสร้างสมการสำหรับทำนายปริมาณโปรตีนและความชื้นของข้าวเปลือก โดยทำการวัดค่าโปรตีนและความชื้นของข้าวเปลือก 33 ตัวอย่าง ที่อุณหภูมิ 4ºC และอุณหภูมิห้อง (25 – 27 ºC) โดยใช้คลื่นแสง NIR ที่ความยาว 730-1100 nm ที่กำเนิดจากเครื่อง AG-RD spectrometer ที่ความถี่ช่องละ 0.5 nm ทำการเปรียบเทียบค่าโปรตีนและความชื้นในตัวอย่างข้าวเปลือกกับค่าที่อ่านได้จากโปรแกรม Unscrambler 9.8 Software (CAMO Software Japan Co. Ltd) ซึ่งให้ผลค่อนข้างดี (ค่า SECV และ R^2 ของโปรตีน = 0.77, 0.96 และสำหรับ SECV และ R^2 ของความชื้นในเมล็ด = 0.43, 0.77 ตามลำดับ) ความชื้นของเมล็ดและค่าต่างๆ ที่อ่านได้ให้ผลไม่แตกต่างกัน (ที่อุณหภูมิ 4ºC มีค่า SECV= 0.89 และ R^2=0.93 และสำหรับที่อุณหภูมิห้องมีค่า SECV = 0.77 และ R^2=0.96) เมื่อทำการคัดเลือกความถี่ที่ดีที่สุดเพื่อให้ได้ค่า R^2 ที่สูงขึ้น พบว่าสามารถเพิ่มค่า R^2 ได้เล็กน้อย โดยมีค่า SECV และ R^2 ของโปรตีน = 0.35 และ 0.83 และมีค่า SECV และ R^2 ของความชื้นในเมล็ด = 0.94 และ 0.94 ตามลำดับ อย่างไรก็ดีเพื่อพัฒนาประสิทธิภาพการทำนาย ควรทำการปรับสภาพตัวอย่างก่อนการวัด เพื่อให้ได้ผลการทดลองที่ดีที่สุด

คำสำคัญ: NIR spectroscopy ความชื้น โปรตีน ข้าวเปลือก

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Introduction

Paddy (*Oryza sativa* L.) sustains two-thirds of the global human population. Japanese rice, or japonica, is a short-grain variety of rice (*Oryza sativa var. japonica*) which is characterized by its unique stickiness and texture. However, during storage, a number of physiological and physicochemical changes occur, which include pasting properties, color, flavor, and composition, result in affecting rice quality (Zhou et al., 2006). Paddy seeds and periods of storage differ in their composition of water, sugar, protein, and lipids differently. Traditional ways to estimate aging of paddy seeds are time-consuming and the sample must be destroyed (Ding JL., 2004). Thus, a quick, accurate, and nondestructive method is needed to classify paddy seed stored for different periods. Near infrared (NIR) spectroscopy provides an alternative, nondestructive technology for measuring constituents of biological materials. Organic molecules have specific absorption patterns in the near infrared region that can be used to determine the chemical composition of the material being analyzed (Williams and Norris, 2001). Collection of near infrared spectra can be collected from the reflectance (NIR) of a sample (Delwiche, 1995, 1998; Williams, 1979). Delwiche et al. (1996) demonstrated that the NIR spectra has been used successfully for the whole-grain milled rice to measure the apparent amylose, protein, whiteness, transparency and alkali spreading value. Kawamura et al. (1999) reported on the analyses of the moisture, protein and amylose contents of rough rice using near-infrared transmission (NIRT) spectroscopy. The aim of this study is to develop robust calibration models that are not affected by temperature for AG-RD spectrometer to predict protein and moisture content in rice.

Materials and Methods

Paddy samples of about 1 kg were obtained for a period of 3 months from September - November 2010. In most cases then the samples were received, placed at a temperature of 4°C, and analyzed the next day. The same samples were left for approximately 6 hours at room temperature before moisture and Spectral measurement for samples at room temperature. Environment temperatures were measured using a thermistor thermometer.

Thirty three paddy samples were measured at cool (4 ºC) and at room temperature (25-27 ºC) over the wavelength range from 730-1100 nm by AG- RD spectrometer at 0.5 nm intervals. Calibrations were developed using Unscrambler 9.8 Software (CAMO Software Japan Co. Ltd) and then they were scrutinized whether there are any tendencies or stratification for each temperature condition.

The samples were placed in the standard sample cells for NIR Measurement. The NIR spectra were acquired in the 730-1100 nm range at 0.5 mm intervals. Calibrations were developed using Unscrambler 9.8 Software (CAMO Software Japan Co. Ltd) over the wavelength of 730-1100 nm. The correlation plots were generated by the same software as indicated. The standard error of cross-validation (SECV) and the coefficient of determination (R^2) were used to assess potential performance of the calibration.

Results and Discussion

Figure 1 and 2 show calibration result for moisture and protein contents, respectively. Although the NIR Spectra were recorded through husk, the results showed that initial calibrations for both moisture and protein content were relatively good (SECV= 0.77, R^2=0.96 and SECV = 0.43, R^2=0.77, respectively. Data not shown) considering that spectra were taken through husk. There is no stratification for both temperature conditions. The statistics for moisture content were SECV= 0.89 and R^2=0.93 for cool and SECV = 0.77 and R^2=0.96 for room while those for protein content were SECV = 0.47 and R^2=0.70 for cool and SECV= 0.42 and R^2=0.62 for room samples. The degree of diffusion of the moisture content is more than protein content. As can be seen from Figures 1 and 2, the stronger calibration and predictions are obtained for moisture while calibration and prediction for protein continued to be weak. However, although moisture calibration and prediction seem to be better than protein, the SEC and SEP for protein is much lower than that of the moisture calibrations. Wavelength selection was then executed in an effort to improve calibration performance and results shows small improvement with R^2 values but the general situation remained the same with moisture calibrations having R^2 of 0.94 and SECV of 0.94 and protein calibrations having R^2 of 0.83 and SECV of 0.35 (data not shown). In order to develop robust calibrations various pretreatment methods will be executed do determine which gives the best results.

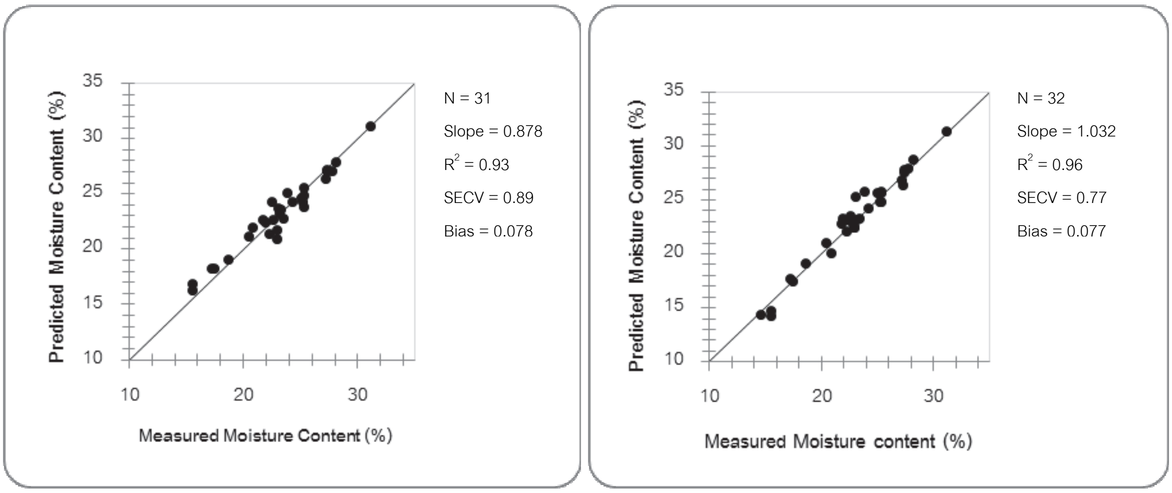

Figure 1. Prediction of cool and room samples moisture contents using above calibration

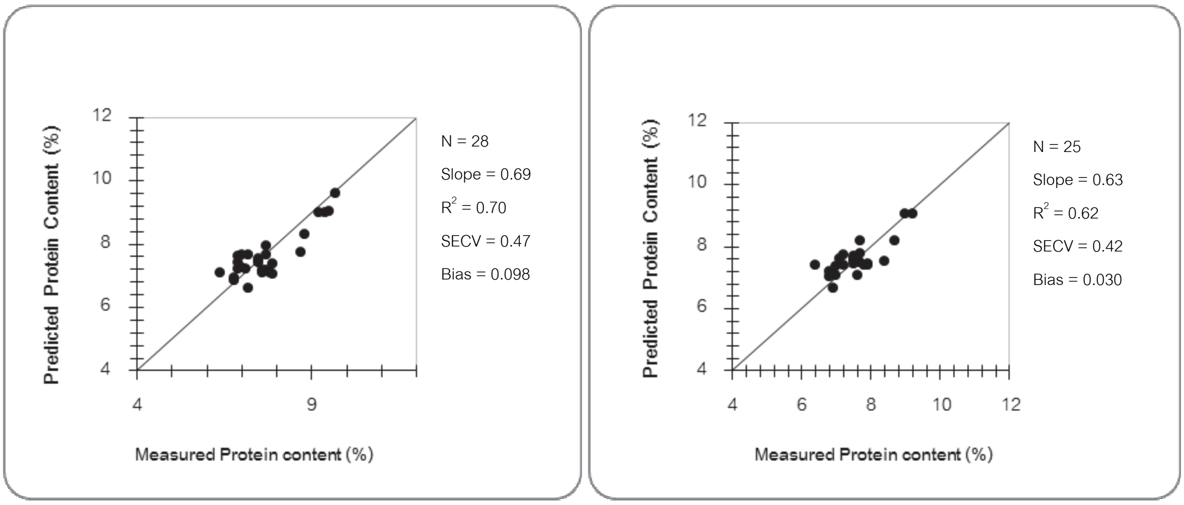

Figure 2. Prediction of cool and room samples protein contents using above calibration

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