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Technical paper

NIR Measurement of Specific Gravity of Potato

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Near infrared (NIR) spectroscopy was investigated as a method for nondestructive measurement of specific gravity of potato. A total of 250 potatoes of three cultivars, Irish-Cobbler, May-Queen and Kita-akari, were used as experiment samples. The NIR spectra (700–1100 nm) of potato samples were acquired by the interactance method and partial least square (PLS) regression analysis was used to develop a predictive model for specific gravity. As a result, the model gave relatively good predictions of the specific gravity, with a correlation coefficient of 0.94 and standard error of prediction of 0.0044 g/cm^3. The results show the potential of the NIR technique as a means for nondestructive measurement of specific gravity of potato with reasonable accuracy.

Keywords: near infrared (NIR) spectroscopy, specific gravity, potato, partial least square regression (PLS)

Introduction

Post-harvest quality evaluation and sorting is required for potato in order to provide reliable and uniform quality to the market place. Similar to many other agricultural products, potato has non-uniform quality and non-uniform maturity at harvest.

One of the properties of potato that could be used as a basis for nondestructive quality evaluation is specific gravity. The relationship between specific gravity and cooking quality of potato has been known for a long time. Zaltzman (1987) reported that Germans were the first to use specific gravity information for evaluating potato quality and developed specific gravity versus starch content tables, and Pohl subsequently calculated the starch content of potato using specific gravity. Other investigators have also reported quality characteristics of potato, including specific gravity and cooking quality (Bewell 1937, Smith *et al.* 1940, Clark *et al.* 1940, Komiyama 2002). They showed the relationship between specific gravity and cooking quality and proposed that specific gravity could be used as a direct and consistent measure of quality characteristics.

In spite of the potential of using specific gravity as a parameter for quality sorting, only limited attempts have been made. Kunkel (1952) reported on mechanical grading of potato according to specific gravity. He developed a method of using a brine solution with a specific gravity of 1.0863. Potatoes were washed prior to entering the brine solution and again after removal to rinse the salt from the surface. The results showed high accuracy of sorting. However, the primary disadvantages with this sorting technique were contamination of the brine solution and the necessity of many fluidized bed media for many levels of quality separation.

Near infrared (NIR) spectroscopy is a useful and nondestructive technique, and has been used to nondestructively determine the sugar content of some agricultural products. Dull *et al.* (1989, 1992) showed that near infrared reflectance in the wavelengths between 800 nm and 1000 nm could be used to determine the sugar content in cantaloupe and honeydew melons. Kawano *et al.* (1992) used a NR spectrophotometer in an interactance mode to measure the sugar content in intact peaches in the spectral region between 680 nm and 1235 nm. They identified four wavelengths related to the sugar content of peaches, with a correlation coefficient (r) of 0.97 and a standard error of prediction (SEP) of 0.5 Brix. Using the interactance mode, similar to Kawano *et al.* (l992), in the spectral region between 400 nm and 1100 nm, Slaughter measured the sugar content of intact peaches and nectarines (1995) and tomatoes (1996). Recently, near infrared spectroscopy has been also used to nondestructively determine the physical properties of some agricultural products. Lu conducted a study to predict the firmness of apples (Lu *et al.*, 2000) and sweet cherries (Lu *et al.*, 2001) with the use of an InGaAs detector in the spectral region between 800–1700 nm. They found that the technique gave good predictions of firmness. The objective of the present study was to investigate near infrared spectroscopy as a means to nondestructively predict the specific gravity of intact potatoes.

Materials and Methods

Materials Three potato cultivars, Irish-Cobbler, May-

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Table 1. Fundamental data of potato samples used.

	Size (g)			Specific gravity (g/cm^3)			R*
	Mean	Range	SD	Mean	Range	SD	
Irish-Cobbler	169.9	96.5-295.1	55.7	1.075	1.057-1.107	0.012	-0.27
May-Queen	176.1	109.5-292.5	41.4	1.076	1.059-1.101	0.011	-0.25
Kita-Akari	145.3	113.1-201.5	21.5	1.093	1.076-1.110	0.007	-0.01

R*:correlation coefficient between size and specific gravity of potato samples.

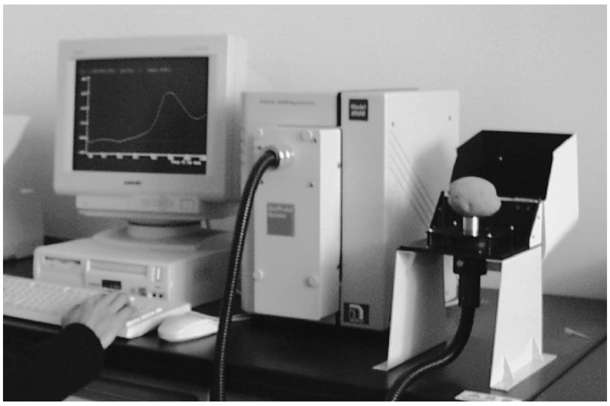

Fig. 1. NIR instrument with fiber optics in interactance mode.

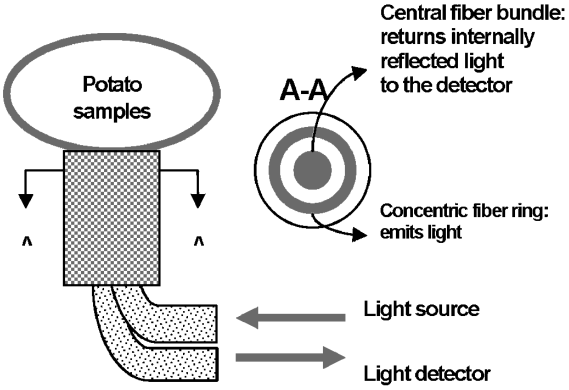

Fig. 2. Conflguration of interactance probe used.

Queen and Kita-akari, were purchased from the Akita fruits and vegetables distribution market. The potato samples were grown at two different locations (Hokkaido and Nagasaki) in Japan. A total of 250 potato samples were used in this study, 100 Irish-Cobbler potatoes (size: M～2L), 100 May-Queen potatoes (size: M～2L) and 50 Kita-akari potatoes (size: M～L). Fundamental data of the potato samples used are shown in Table 1.

Specific gravity Following spectral measurement, the specific gravity of each sample was measured using specific gravity measurement equipment (SHIMADZU, SGM-300P) based on the principle of liquid displacement. Intact potato samples were first weighed in air and then forced into a liquid (distilled water) by means of sinker thread, and a second weight reading of the potato submerged in liquid was obtained. The specific gravity was calculated as follows:

$$\text{specific gravity} = \frac{\text{weight in air} \times \text{specific gravity of liquid}}{\text{weight in air} - \text{weight in liquid}}$$

Near infrared spectra From the viewpoint of practical use, the interactance model was adopted to measure near infrared (NIR) spectra of intact potato samples. A spectrophotometer (NRSystems model 6500) equipped with a fiber optic probe is shown in Fig. 1. The fiber optic probe consisted of a central bundle (7.6 mm in diameter) of Schott glass fibers surrounded by a 0.64 mm wide concentric ring of Schott glass fibers with an outside diameter of 19 mm, as shown in Fig. 2. The outer ring of fibers was separated from the central bundle by a 5 mm thick metal barrier. To collect the optical spectrum, an intact potato was placed against the optical probe with the center of gravity on the center of the probe. Monochromatic light emitted by the outer ring of fibers entered and "interacted" with the tissue. Some of the nonabsorbed light was internally diffuse-reflected and exited the intact potato and was collected by the central bundle of optical fibers.

The NIR spectra (400–1100 nm) were measured as absorbance log (1/R) at 2 nm increments. A 2.5 mm thick ceramic plate was used as the standard optical reference. Each spectrum was an average of 32 scans and one spectrum was obtained per potato sample. Prior to spectral measurement, the samples were placed in a measurement room (20℃) for 24 hours to ensure each sample was the same temperature during spectrum acquisition.

Calibration and validation A total of 250 potato samples were separated into two groups; 150 samples for calibration and 100 samples for validation. Statistical specific gravity values of the samples selected for the calibration and validation sample sets are shown in Table 2. The calibration and validation sample sets covered similar means and standard deviations for specific gravity. Calibration and validation were performed using the Unscrambler software (Ver.7.6, Camo ASA, Norway). Potato samples in the calibration group were used to establish multivariate equations between spectral data and laboratory reference values, and samples in the validation group were used to evaluate these calibration equations. In calibration, equations were developed using modified PLS

Table 2. Mean, range and standard deviation (SD) of specfic gravity of potatoes for calibration and validation sample sets.

	Calibration (n=150)			Validation (n=100)		
	Mean	Range	SD	Mean	Range	SD
Specific gravity (g/cm^3)	1.079	1.057-1.110	0.013	1.079	1.060-1.104	0.013

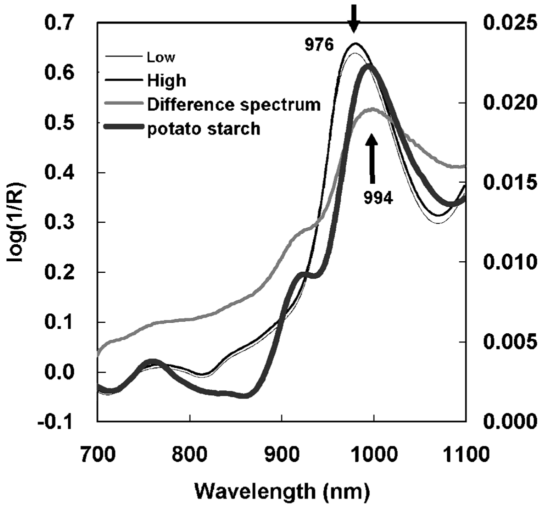

Fig. 3. Average NIR spectra for two specific gravity classes (low and high) of potatoes and its difference spectrum (high-low).

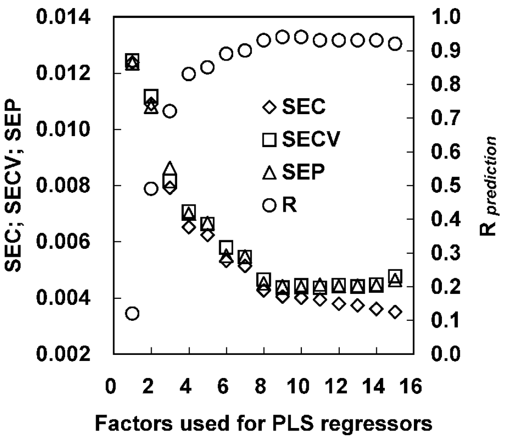

Fig. 4. Perfomance values of PLS regression analysis for specific gravity of potatoes based on raw NIR spectra.

(partial least squares) regression based on raw spectra or other spectra after preprocessing. Range normalization, first derivative, second derivative, multiplicative scatter correction (MSC) and orthogonal signal correction (OSC) were used to remove the variation in spectra caused by unknown sources that tend to increase errors in calibration models. The PLS regression analysis was performed using the spectra from 700 to 1100 nm. The optimum number of PLS factors was determined by cross validation, that is, the best calibration equations were judged by the lowest standard error of cross-validation (SECV). After equations were established, samples in the validation group were used to assess the prediction accuracy of the calibration equation by the standard error of performance (SEP), correlation coefficient (R), and bias.

Results and Discussion

NIR spectra and difference spectrum Potato samples were arranged in order of specific gravity for each cultivar, and then divided into the first half of potato samples and the latter half of potato samples. Samples in the first half of all cultivars were combined into a low class and samples in the latter half of all cultivars were combined into a high class. Figure 3 shows the average near infrared spectra (700–1100 nm) for the two specific gravity classes (low and high) and its difference spectrum (high-low). The two average spectra were rather smooth across the entire spectral region and had two broadband peaks around 760 nm and 976 nm related to water in the potatoes. Potatoes in the high specific gravity class had higher absorption across the entire spectral region. This fact could also be clearly seen in the difference spectrum, because the difference spectrum had positive values across the entire spectral region. Further, we also found that the difference spectrum had a broadband positive peak around 994 nm, which could be attributed to O-H stretching second overtone (Osborne, 1993), and the peak could be related to starch by means of comparing absorption band of potato starch as shown in Fig. 3. The above observation appears to indicate that information about specific gravity is included the NIR spectra measured by the interactance method.

Calibration and validation for specific gravity PLS regression analysis was performed based on the specific gravity and raw NIR spectra (700–1100 nm) of the calibration and validation sample groups. Figure 4 shows that NIR performance values were influenced by the number of factors of the calibration model. As the number of factors of the calibration model increased, NIR performance values of SEC (standard error of calibration) decreased. The NIR performance values of SECV (standard error of cross validation: derived from internal validation during the calibration process) decreased from an initial value of about 0.210 to about 0.004 with 9 factors. Thereafter the values of SECV slowly increased again. The calibration model with 9 PLS factors was obtained from the calibration sample sets. The other NIR performance value of SEP (standard error of prediction: calculated from validation, using independent validation samples) decreased from the initial factor to the 9th factor as with SECV. Thereafter, the value of SEP increased slowly and indicated an "over fit" when the number of factors of the calibration model increased. Thus, we confirmed that the optimal number of factors to predict specific gravity using raw NIR spectra was 9. Figure 5 shows the calibration and prediction results of specific gravity of potato. The correlation coefficient of calibration was as high as 0.95, with a standard error of calibration (SEC) of 0.0041 g/cm^3. When the calibration model was used to predict the other independent validation samples, good predictive results were obtained (correlation coefficient of 0.94, standard error of prediction of 0.0044 g/cm^3). As an index for determining the validity of the measurement accuracy of a calibration model, the RPD (ratio of standard deviation of reference data in prediction sample set to SEP) is usually utilized (Williams, 2001). A RPD value of 2.5–3.0 is regarded as adequate for rough screening and a value of above 3.0 is regarded as satisfactory for screening. In this study, a RPD value of 3.0 was obtained, thus the calibration model is considered to have suitable accuracy for measurement of the specific gravity of potato.

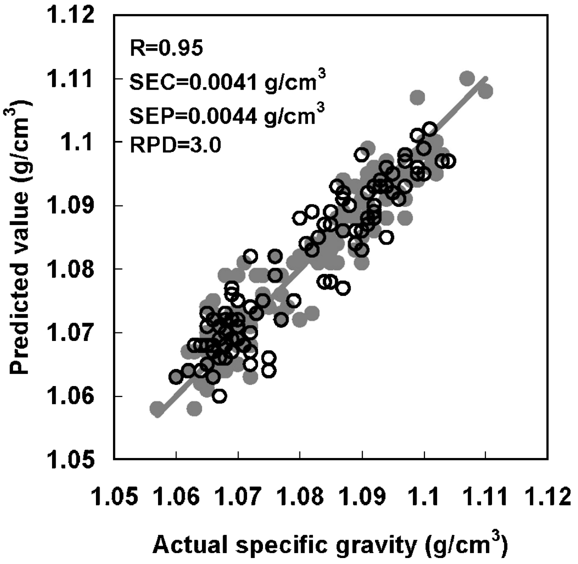

Fig. 5. Scatter plots of actual specific gravity of potato and predicted values.

Loading weights of the PLS calibration model Loading weight can be used to discuss the contributions of individual wavelengths to the PLS calibration model, because loading weight has some characteristic peaks and troughs, indicating which wavelength range was important for the calibration model (Chen, 1999, Williams, 1996, Martens, 1989). Figure 6 shows the first six loading weights of the PLS calibration model for specific gravity

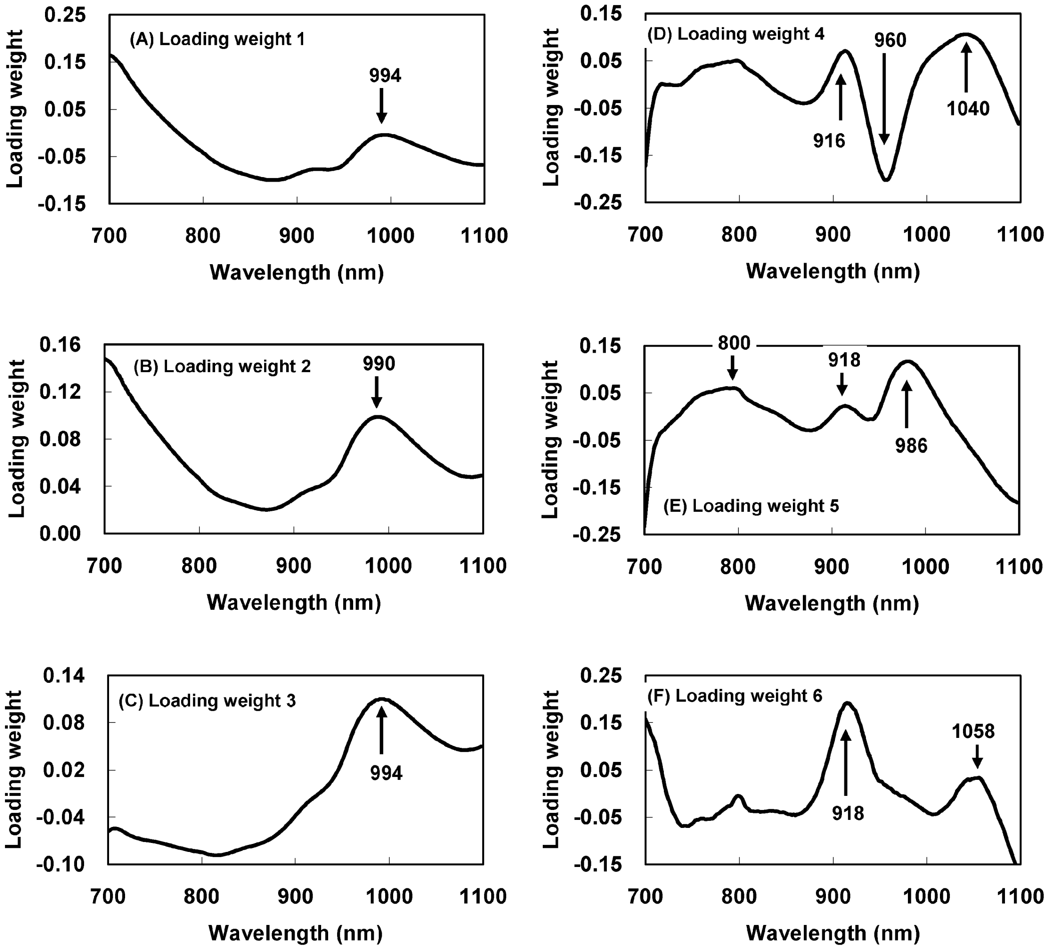

Fig. 6. loading weights for first six factors in PLS calibration model.

of potato. The first three loading weights were similar, and had a broadband positive peak around 990 nm attributed to O-H stretching second overtone related to starch. The fourth loading weight had a positive peak around 916 nm attributed to C-H stretching third overtone related to starch or protein and a positive peak around 1040 nm attributed to the combination of stretching and deformation of C-H bonds related to lipid. In addition, the fourth loading weight had another negative characteristic peak around 960 nm attributed to O-H stretching second overtone related to water in potato. The fifth loading weight showed a positive peak around 986 nm attributed to O-H stretching second overtone related to starch, a small peak around 918 nm attributed to C-H stretching third overtone related to starch or protein and a broadband positive peak around 800 nm attributed to N-H stretching third overtone related to protein. The sixth loading weight had a positive peak around 918 nm attributed to C-H stretching third overtone related to starch or protein and a small peak around 1058 nm attributed to N-H stretching second overtone related to protein. From these observations, we believe that the PLS calibration model for the specific gravity of potato was established based on the absorption bands of potato components, especially starch because the first three loading weights showed absorption bands of starch. That is to say, the calibration model mainly utilized characteristic absorption band of starch. This fact may be attributed to the high correlation between the specific gravity and starch content of potato (Nagata, 1956).

Table 3. Correlation coefficients between specific gravity of potatoes and scores for factors in LPS calibration model.

PLS factors	Correlation coefficients
1st	0.22
2nd	0.40
3rd	0.60
4th	0.30
5th	0.28
6th	0.25
7th	0.14
8th	0.23
9th	0.09

In addition, we also observed that the third loading weight had a very similar shape to the difference spectrum shown in Fig. 3. This demonstrates that the third factor of the PLS calibration model provides more information about the specific gravity of potato, as confirmed in Table 3. Table 3 showed the highest correlation coefficient between specific gravity and score of the third factor in the PLS calibration model.

Effect of preprocessing of NIR spectra on PLS calibration model In order to investigate whether preprocessing for raw NIR spectra could provide more accurate measurements, preprocessing such as range normalization, first derivative, second derivative, multiplicative scatter correction (MSC) and orthogonal signal correction (OSC) was performed on the raw spectra (700–1100 nm), and predictions for specific gravity were examined. The calibration and prediction results are shown in Table 4. Similar results were obtained when the NIR spectra after these preprocessing techniques were used to predict the specific gravity of potatoes. Normalization is often used to correct spectra for indeterminate path length when it cannot be measured and the MSC or OSC methods are mainly used for removing the effects of light scattering on spectra. In the present case, we found that these preprocessing techniques led to fewer factors in the calibration models except range normalization, but did not improve the accuracy of predictions of specific gravity. Therefore, reprocessing of NIR spectra was not necessary for the present case.

Conclusions

Based on the results of this study, the following conclusion can be made:

NIR spectroscopy had reasonable accuracy in measuring the specific gravity of intact potato with a correlation

Table 4. NIRB performance values for specific gravity (g/m^3) of potatoes.

Preprocessing-method	Factors	Calibration		Validation		Prediction			
		R cal	SEC	R val	SECV	R pred	SEP	Bias	RPD
Raw spectra	**9**	**0.95**	**0.0041**	**0.94**	**0.0044**	**0.94**	**0.0044**	**-0.00003**	**3.0**
Normalization	**9**	**0.95**	**0.0041**	**0.93**	**0.0045**	**0.94**	**0.0044**	**0.00034**	**3.0**
First derivative	**7**	**0.94**	**0.0043**	**0.93**	**0.0046**	**0.93**	**0.0047**	**0.00019**	**2.8**
Second derivative	**7**	**0.95**	**0.0041**	**0.94**	**0.0044**	**0.93**	**0.0045**	**0.00019**	**2.9**
MSC	**7**	**0.94**	**0.0042**	**0.94**	**0.0045**	**0.93**	**0.0045**	**0.00031**	**2.9**
OSC	**8**	**0.94**	**0.0042**	**0.93**	**0.0045**	**0.93**	**0.0045**	**0.00005**	**2.9**

R cal, correlation coefficient of calibration; SEC, standard error of calibration;
R val, correlation coefficient of cross-validation; SECV, standard error of cross-validation;
R pred, correlation coefficient of prediction; SEP, standard error of prediction;
RPD, ratio of standard deviation of reference data in prediction sample set to SEP

coefficient of 0.94 and a standard error of prediction (SEP) of 0.0044 g/cm^3.

The calibration model developed for determining the specific gravity of potato mainly utilized the characteristic absorption band of potato starch.

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