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Towards on-line prediction of dry matter content in whole unpeeled potatoes using near-infrared spectroscopy

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ABSTRACT

Prediction of dry matter content in whole potatoes is a desired capability in the processing industry. Accurate prediction of dry matter content may greatly reduce waste quantities and improve utilization of the raw material through sorting, hence also reducing the processing cost. The following study demonstrates the use of a low resolution, high speed NIR interactance instrument combined with partial least square regression for prediction of dry matter content in whole unpeeled potatoes. Three different measuring configurations were investigated: (1) off-line measurements with contact between the potato and the light collection tube; (2) off-line measurements without contact between the potato and the light collection tube; and (3) on-line measurements of the potatoes. The offline contact measurements gave a prediction performance of R^2=0.89 and RMSECV=1.19. Similar prediction performance were obtained from the off-line non-contact measurements (R^2=0.89, RMSECV=1.23). Significantly better (p=0.038) prediction performance (R^2=0.92, RMSECV=1.06) was obtained with the on-line measuring configuration, thus showing the possibilities of using the instrument for on-line measurements. In addition it was shown that the dry matter distribution across the individual tuber could be predicted by the model obtained.

1. Introduction

The potato processing industries, and especially the frying and starch industries, are heavily dependent on reliable measurements of dry matter content. This is an important quality parameter frequently used to determine both the cost of the raw material and, most importantly, the subsequent choice of processing parameters. Today, most processing plants adjust their processes based on dry matter content predicted by simple gravimetric methods, which are based on the density of the potatoes [1,2]. These predictions are based on batch samples (typically 5 kg samples), which implies that any process adjustments are based on average dry matter content of a small subset, and not of a whole batch of potatoes. The variation within a crop is then not taken into account. This variation is found to be significant, and it depends on factors such as growing conditions and choice of cultivar [3,4]. The ability to accurately predict the dry matter content, and the resulting possibilities for continuous sorting, would allow for a more uniform stream of raw material. This is expected to lead to easier processing and a significant decrease in waste quantities.

Near-Infrared (NIR) spectroscopy is a frequently used tool for rapid and reliable prediction of quality parameters in a wide variety of foods [5,6]. This technology can then give input for devices for sorting of both animal and vegetable based foodstuff [6–8]. NIR measurements with subsequent sorting is usually based on the chemical composition of the foodstuff, but it has also been used for more physical parameters such as the gross meat content of intact crabs [9].

NIR analyzes have been extensively studied for potatoes in recent years. These studies have, however, often been restricted to homogenized samples like potato pulp, sliced potatoes and cooked potato mash [10]. The prediction of dry matter content in such samples is highly accurate, as the water is sensitively probed [10]. Haase and co-workers [11,12] obtained a coefficient of determination (R^2) around 0.98 for prediction of dry matter content of potato pulp. Also the starch content, which is closely correlated with dry matter content in potatoes, can be predicted with high accuracy in homogenized samples using NIR. Minor constituents like sugars are generally reported to yield lower prediction performance [10], although some authors have achieved decent predictions (R^2=0.82) of total reducing sugar content in homogenized

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samples [13].

Despite the promising results of using NIR for prediction of dry matter in homogenized samples, the use of NIR on whole unpeeled potatoes is only infrequently encountered in the literature. Transmission studies performed by Dull and coworkers [14] paved the way for investigation of whole unpeeled potatoes, and moderate prediction performance (R^2=0.84) was obtained for dry matter of intact potatoes. Subedi and Walsh [15] obtained similar predictions (R^2=0.85) of dry matter in their NIR analysis of whole potatoes, but in reality only a small cube of potato tissue directly below the measured area was used for reference analysis. Another approach that has shown decent performance is the use of NIR spectroscopy for prediction of the specific gravity (i.e the density) of potatoes [16]. The drawback with this approach is the conversion of specific gravity to dry matter content. The equations used for this conversion are often old and many different models exist, indicating that the relation between specific gravity and dry matter content might depend on several different factors [17].

In all above-mentioned studies, high resolution laboratory instruments were utilized, lacking the speed necessary for on-line industrial applications. The present authors recently showed that a rapid NIR interactance system of low spectral resolution (15 NIR channels) can be used for predicting dry matter (R^2=0.95) in whole unpeeled potatoes off-line [4]. The light penetration depth in intact potatoes was found to be approximately 20 mm. On the other hand, when employing a commercial on-line NIR interactance imaging system, lower prediction performance (R^2=0.83) was obtained [4]. The lack in performance for measurements of whole unpeeled potatoes, with the latter instrument, can most likely be ascribed to shallow light penetration ($<$ 10 mm) into the potato combined with the heterogeneous distribution of dry matter content within the potato tuber [18–20]. The dry matter content may differ significantly from the outer to the inner part of the potato tubers [21]. Similar results were reported for on-line studies of sliced samples (R^2=0.85) [15]. Despite recent efforts, there is still no commercially available system for on-line prediction of dry matter in whole unpeeled potatoes.

In the present study, a rapid prototype high speed, low resolution NIR interactance system (described in [4, 5]) is demonstrated. The aim of the current study was to investigate and evaluate further use of this instrument for online prediction of dry matter content in whole unpeeled potatoes, using three different sampling configurations: (1) off-line measurements with contact between the potato and the light collection tube; (2) off-line measurements without contact between the potato and the light collection tube; and (3) on-line measurements of the potatoes. The impact of the intra tuber dry matter gradient on the prediction performance was also investigated, as this was suspected to affect the prediction of dry matter content in samples moving past the detector.

2. Materials and methods

2.1. Dataset and sample preparation

A total of 240 potatoes from 7 different potato cultivars were obtained from either commercial suppliers or local potato processing industry. An overview of the cultivars and number of samples are provided in Table 1. All samples were stored at 4 °C prior to analysis. Samples were cleaned by hand in tap water and equilibrated (16 h) to ambient temperature (18 °C), also allowing the outer skin to dry prior to spectral acquisition.

2.2. Spectral acquisition

A prototype NIR interactance instrument was used for spectral acquisition [5]. Whole potato tubers were illuminated with two 50 W halogen bulbs (Osram, Augsburg Germany) and backscattered light was collected through a collection tube. The instrument was equipped with a detector recording 30 equally spaced channels from 449 to 1040 nm [5], thus recording both visible and near infrared light. In this study the 15 channels from 760 to1040 nm were used, thus excluding the visible part of the recorded spectrum. The NIR measurements were performed in three different ways: (1) the potato was placed in direct contact with the light collection tube of the NIR instrument, henceforth denoted “off-line contact measurements”. This collection geometry has been previously studied [4]; (2) the potato was placed approximately 10 mm below the light collection tube of the NIR instrument, henceforth denoted “off-line non-contact measurements”. This configuration was used to mimic the optical path length encountered in typical on-line situations; and (3) on-line collection of spectra of potatoes moving along a conveyor belt below the collection tube, henceforth denoted “on-line measurements”.

For both off-line contact and non-contact measurements a collection time of 2 s was set. Measurements were performed in triplicate, rotating the sample 60° in the horizontal plane, between each measurement. Spectra were acquired from the center of the longitudinal axis, which is by others found to be the location with dry matter content closest to the average of the potatoes [21]. On-line measurements were performed by sending the potatoes along a conveyor belt moving at 15 cm/s with the detector mounted directly above the conveyor belt. Each potato was exposed to the light for about 1/3 of a second. The sampling rate for the spectrophotometer was 80 spectra per second, and each measurement lasted for 5 seconds. Each moving potato was measured in triplicate, but was not rotated between measurements. They were placed on a small metal ring to stabilize them and prevent them from rolling around on the conveyor belt.

2.3. Reference analysis

Each individual potato tuber was carefully grated into strips (cross section of 2 × 3 mm) with a bench top grater (Hallde RG-

Table 1
An overview of the samples used (DM=dry matter content).

Cultivar:	Min. DM	Average DM	Max. DM	St.Dev DM	No. of samples	Skin color	Flesh color
Asterix	14.7	19.1	23.5	2.0	30	Red	Light yellow
Bruse	25.4	28.1	31.5	1.3	40	Red	Light yellow
Fakse	17.7	20.3	22.6	1.3	40	Yellow	Light yellow
Folva	17.1	20.3	23.8	1.4	30	Yellow	Light yellow
Mandelpotet	21.9	25.9	29.3	2.1	30	Yellow	Yellow
Saturna	21.8	25.4	28.3	1.4	40	Yellow	Light yellow
Sava	18.2	20.4	22.4	1.1	30	Yellow	Yellow
All samples	**14.7**	**23.0**	**31.5**	**3.7**	**240**	**-**	**-**

100, AB Hällde Maskiner, Sweden). Three sub-samples (20 ± 1 g) of each potato tuber were immediately placed in aluminum pans and dried for 48 h at 105 °C in a forced fan oven. Dry matter percentages were calculated based on the weight before and after drying. The standard error of the reference method (S_{ref}) was calculated by the following Eq. (1):

$$S_{ref} = \sqrt{\frac{\sum_{i=1}^{I} s_i^2}{I \cdot N}} \quad (1)$$

Here, s_i denotes the standard deviation for each sample, I denotes the number of replicates and N denotes the number of samples.

2.4. Data processing

Spectra from off-line contact and off-line non-contact measurements were pre-processed using an in-house MATLAB routine (MATLAB, V.7.10, The MathWorks, Natick, MA). Averaging of replicate spectra from each sample was performed, and all spectra were log-transformed into apparent absorbance values. Spectra from the on-line measurements were processed by another in-house built MATLAB routine, separating potato spectra from conveyor belt spectra. NIR spectra from the conveyor belt differed from spectra obtained from potatoes. Separation of the two types of spectra could be based on intensity differences in the raw spectra, observed at four different wavelengths (i.e. the intensity of 800 nm had to be greater than the intensity of 760 nm and the intensity difference between 880 nm and 820 nm had to be greater than 350). Finally, an average of the three replicate measurements from each potato was calculated.

In addition to the averaged spectra representing a whole potato tuber, the MATLAB routine provided the individual spectra from each potato tuber. Each individual spectrum represented a movement of 2–3 mm along the axis of the potato. These were used for calculation of the gradient in dry matter content along the potato.

Further processing was performed using the Unscrambler X software (V.10.2, CAMO PROCESS AS, Oslo Norway). The standard normal variate (SNV) transformation [22] was applied to spectra from both types of measurements. Subsequently, regression models were developed using Partial Least Squares (PLS) regression [23], with the dry matter values determined by oven drying used as reference values. The optimal number of PLS factors was determined by leave-one-out cross validation. Root Mean Square Error of Cross Validation (RMSECV) was estimated by the following Eq. (2):

$$RMSECV = \sqrt{\frac{\sum_{i=1}^{I} (\hat{y}_i - y_i)^2}{I}} \quad (2)$$

where i denotes the samples from 1 to I, y_i and $\hat{y}_i$ denotes the reference value and the predicted value, respectively. Principal Component Analysis (PCA) was performed in the Unscrambler X software to elucidate the variation within the dataset.

Analysis of variance of the cross validation (CVANOVA) [24] were performed, including a two-way ANOVA and pairwise comparison (Tukey's), using MiniTab (MiniTab v16, MiniTab Inc. USA), allowing significance testing of model differences.

3. Results and discussion

The dataset comprised 240 potatoes of 7 different cultivars. An overview of the samples is provided in Table 1. The dry matter range spanned from 14.7 to 31.5%, thus covering most of the natural variation found in potatoes [19]. The standard error of the reference method was estimated to be 0.18%.

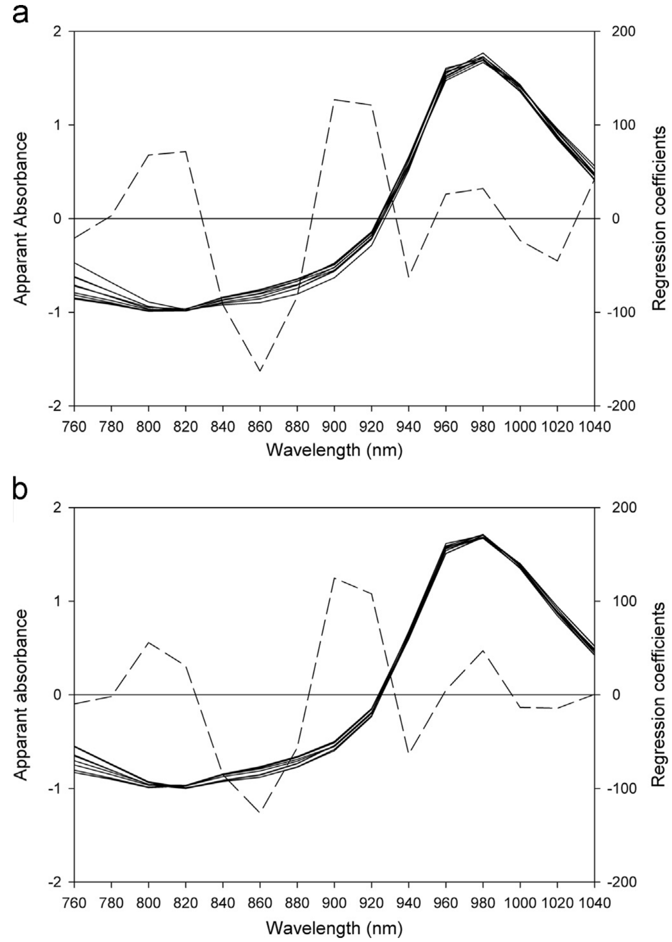

Fig. 1. Example spectra (solid lines) and regression coefficients (dotted lines) for the models obtained from the off-line contact (a) and off-line non-contact (b) measurements. Spectra shown are SNV-transformed apparent absorption spectra. The models obtained from contact and non-contact measurements are both made with 5 PLS factors.

3.1. Off-line contact and non-contact measurements

Spectra recorded using the off-line contact configuration gave a PLS regression model with R^2 value of 0.89 and an RMSECV value of 1.19 (5 PLS factors). SNV-transformed spectra of the potatoes along with regression coefficients of the 5 factor PLS model are shown in Fig. 1a. When examining the regression coefficients, it became evident that the main contribution to the regression model comes from a region around 890-930 nm. A smaller contribution can be found around 960-980 nm. The region around 960 nm is known to contain the second overtone from the O–H bond in water molecules [25]. This may seem contradictory, but the C–H bond in starch may, according to Williams and Norris [25], have a strong absorption band at 979 nm. This may explain the positive contribution from this area. 878 and 901 nm are also pointed out as two starch absorption bands by Williams and Norris [25]. The regression coefficients are very similar to those found by others [15], except that they are shifted about 30 nm to the right in relation to the spectra. Subedi and Walsh [15] used the second derivative of absorption spectra, rather than SNV-transformed absorption spectra, which may explain the shift in regression coefficients. The regression coefficients are also almost identical to those found in a previous study by the current authors [4]. The

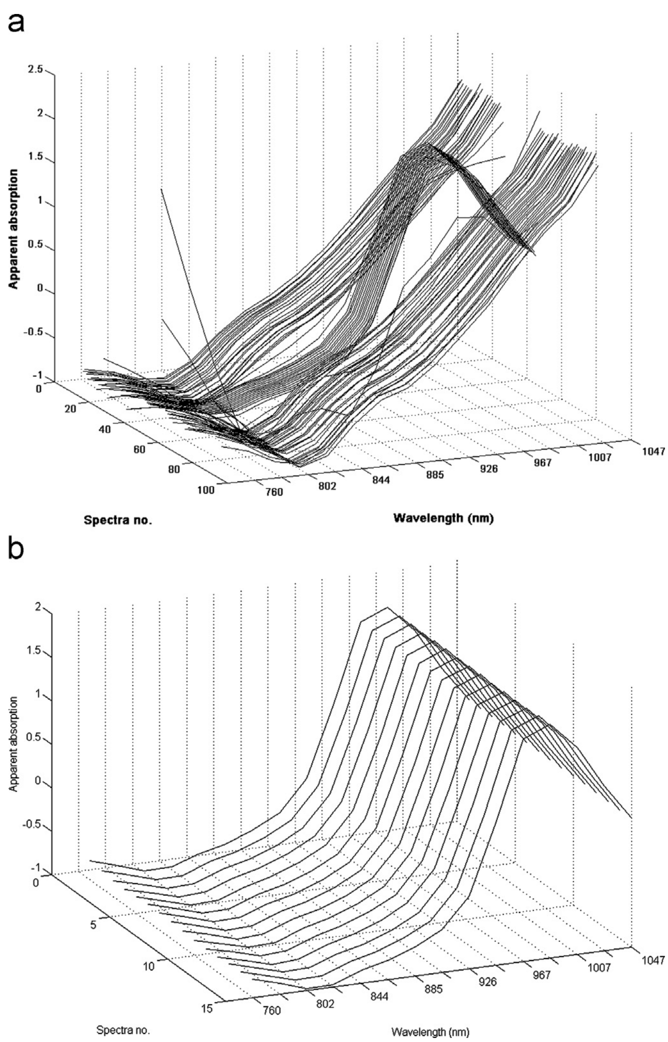

Fig. 2. (a) A section of the recording from an on-line measurement of a potato. Spectra with a peak at 950–990 nm represent the potato, the rest of the spectra represent the conveyor belt. All spectra seen are SNV-transformed. The sample shown is from the cultivar Asterix. (b) Spectra remaining after removal of all spectra representing the conveyor belt.

prediction performance, however, is slightly lower than what was achieved in the previous study, which may be ascribed to a larger dataset and different selection of cultivars in the current study.

The spectra obtained from the off-line non-contact configuration yielded a prediction performance comparable to the off-line contact method, with $R^2=0.89$ and RMSECV$=1.23$ (5 PLS factors). The difference in performance was not significant ($p=0.482$). SNV-transformed spectra and regression coefficients can be seen in Fig. 1b. It should be noted that the regression coefficients are found to be very similar to those found for the off-line contact measurements, which indicates that the non-contact configuration does not significantly alter the output of the NIR measurements. The ability to perform non-contact measurements is essential in order to develop a procedure for on-line measurements.

3.2. On-line measurements

On-line measurements require that the sampling procedure can distinguish between the samples and the conveyor belt. One way to do this is to utilize the spectral difference between the background (e.g. the conveyor belt) and the sample. In Fig. 2a a section of the recording, before the threshold was applied, can be seen. It contains both the potato spectra and the conveyor belt

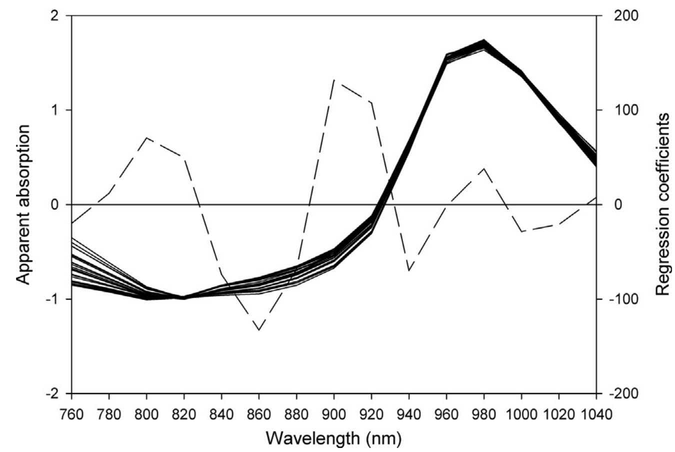

Fig. 3. Spectra (solid line) from potatoes moving past the detector. Each spectrum shown contains the averaged spectra from one sample, and is SNV-transformed apparent absorption spectra. Regression coefficients (dotted line) are shown for the prediction model (6 PLS factors) obtained for prediction of dry matter content in potatoes moving along conveyor belt.

spectra (both SNV-transformed). The potato is represented by the spectra with a clear peak around 970 nm. NIR spectra after removal of the conveyor belt-spectra can be seen in Fig. 2b. All spectra extracted from one potato tuber were averaged and used for PLS regression. A regression model based on the on-line measurements gave good prediction performance ($R^2=0.92$, RMSECV$=1.06$, 6 PLS factors). The model obtained from the on-line measurements was significantly better than the model from the off-line non-contact measurements ($p=0.038$), but not significantly better than the model from the off-line contact measurements ($p=0.362$). Example spectra from the on-line measurements, along with the regression coefficients of the corresponding PLS model, are shown in Fig. 3. The spectra and the regression coefficients do not differ much from the ones acquired from the off-line results. All regression results are summarized in Table 2.

To evaluate if the extraction criterion was correct and if the number of spectra extracted from each potato tuber could be reduced, PLS models were made extracting fewer spectra from each sample. First, a model was made using only the three spectra from the middle of each sample. This model had a significantly ($p=0.036$) lower prediction performance ($R^2=0.89$ and RMSECV$=1.25$) than the one using all spectra from each potato tuber. Secondly, two spectra from each end of the potato tuber were removed to see if removal of potential interference from the conveyor belt and reduced light scattering effects caused by the curvature of the potato tuber would improve the prediction performance. This also gave a model with slightly lower, but not significantly lower ($p=0.926$), prediction performance ($R^2=0.91$ and RMSECV$=1.11$) compared to the model using all spectra. This may also indicate that the threshold used to distinguish between

Table 2
An overview of the performance of the different regression models obtained.

Measuring configuration:	R^2	RMSECV (%)	No. of PLS- factors
Off-line contact[a,b]	0.89	1.19	5
Off-line non-contact[b]	0.89	1.23	5
On-line[b]	0.92	1.06	6
On-line – 2 end-spectra removed[b]	0.91	1.11	6
On-line – 3 middle spectra[a]	0.89	1.25	6

[a] Measuring configurations not shearing a common letter show significantly different prediction performance.
[b] Measuring configurations not shearing a common letter show significantly different prediction performance.

the sample and conveyor belt worked as intended. This shows that a further reduction in the number of extracted spectra by removing spectra from each end of the sample will remove information rather than noise.

The average size of the potatoes used in this study was 50 mm across the shortest axis. At the conveyor belt speed used, this should theoretically result in an average of 20 spectra per potato using the current equipment. After extraction of the sample spectra from the conveyor belt, an average of 15–17 spectra were left, hence further indicating that the threshold was effectively removing enough to avoid interference from the conveyor belt and the outermost ends of the potato.

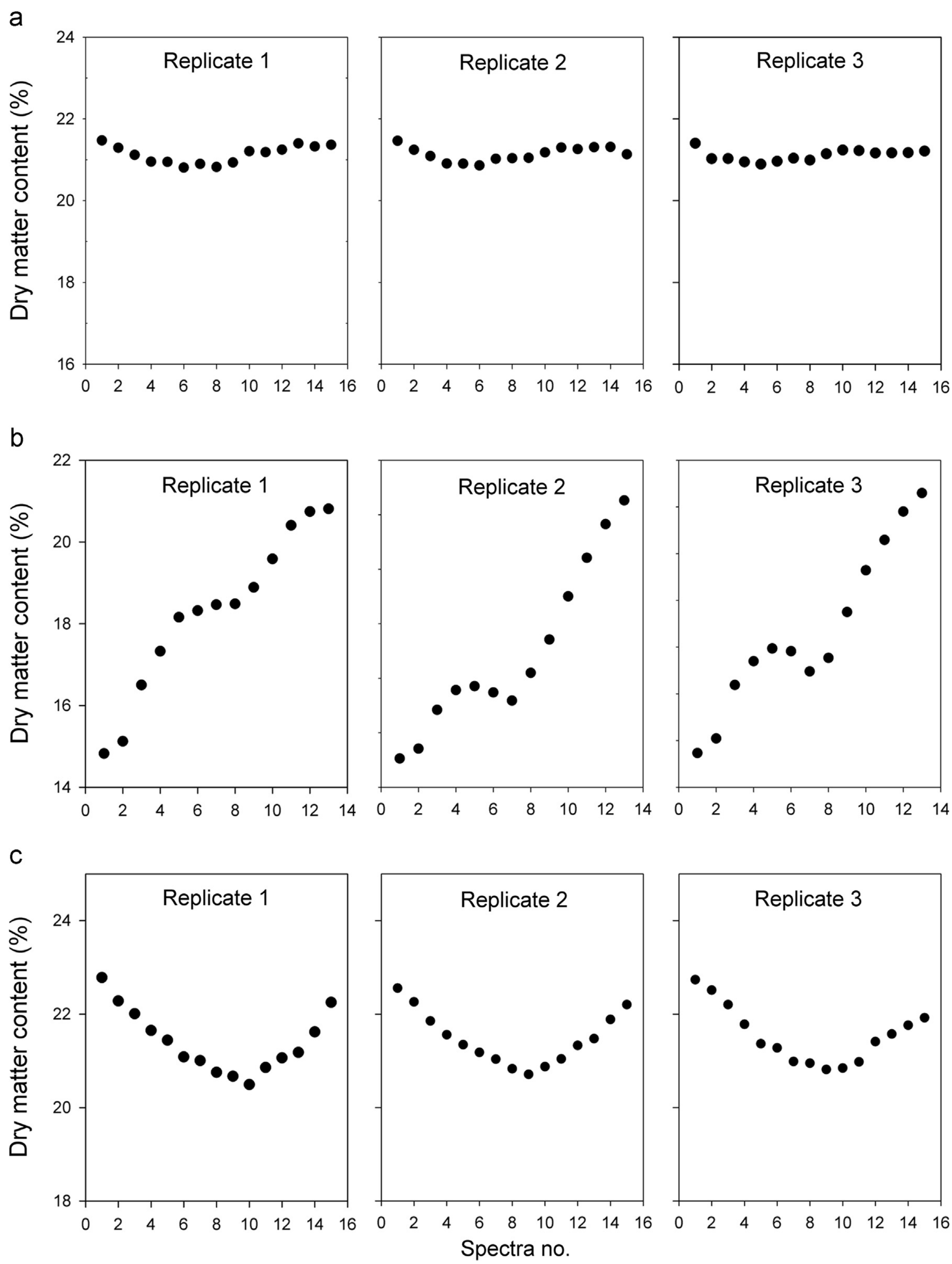

Fig. 4. Three different patterns emerged when dry matter content was predicted from the individual spectra recorded from a sample. Note that three replicates are shown side by side. (a) a sample with rather homogenous dry matter content, (b) increasing (or decreasing, if potatoes was turned the other way before measurement) dry matter along the potato length, (c) potatoes with lower dry matter content at the center, and higher dry matter content in the periphery.

Given the above-mentioned measurement conditions, each individual NIR spectrum will represent 2–3 mm of movement along the potato axis. This could allow for prediction of internal dry matter differences along the main axis of the potato. Thus, the individual NIR spectra from each potato were extracted, and dry matter content of each spectrum was predicted using the PLS model established with the averaged spectra from the on-line measurements, as described above.

It should be noted that the PLS regression used for this was made based on spectra and dry matter content values averaged over whole potatoes. The dry matter along the potato axis may not fully correspond to the average value in the potato [21], hence values predicted for individual spectra along the potato may not fully correspond to the actual value found in the potato. The interrelation between the different spectra should, however, be correctly predicted. The variation in dry matter content across the potatoes fell mainly into three different categories. Examples of internal dry matter distributions along the main axis of potatoes are provided in Fig. 4. The first category consisted of potatoes with nearly constant dry matter content across the potato axis. A prediction example of this is shown in Fig. 4a. Note that three replicates of the same potato are shown side by side. The second category consisted of the potatoes where the dry matter content increased from one end of the measurement to the other. Whether this is seen as decrease or increase depends on the direction of measurement, as can be seen in Fig. 4b. The trend shown in Fig. 4b is believed to be the gradient found along the longitudinal axis (perpendicular to equatorial axis). The third category contained potatoes where the dry matter decreased towards the center, but then increased again when approaching the other end of the potato, shown in Fig. 4c. This is believed to be the dry matter gradient from the stem end towards the bud end of the potato (longitudinal axis). The two different dry matter gradients shown in Fig. 4a and b were representative for most of the potatoes analyzed, and the results are in good compliance with the findings of Peiris and co-workers [26]. This relationship is also established by other authors [18, 21]. For some potatoes, however, peculiar and deviating results were obtained, which also was clear from the specific prediction errors obtained from the software. This might indicate that the shape of the potato was irregular and hence not allowing accurate prediction, or that the water gradient within the tuber may not be constant for all potatoes. Overall, the internal gradients and the corresponding interpretations serve as a strong indication that the NIR approach is feasible for internal dry matter content predictions.

3.3. General discussion and further development

The off-line contact measuring configuration, described in the section *Off-line contact and non-contact measurements* (summary given in Table 2), should theoretically give the best prediction result, due to the elimination of all surface reflection and stray light of the measurements. The off-line non-contact and the on-line measurements do allow some surface reflection and stray light to be collected. The regression model shows, not surprisingly, a slightly, but not significantly lower prediction performance for the off-line non-contact compared to the off-line contact measurements. However, the on-line measurements provided a significant increase in prediction performance compared to the off-line non-contact configuration, but the PLS model needed one additional PLS factor, as described in the section *On-line measurements*. Since the dry matter content varies along the length of the tuber, the on-line measurements might therefore give a better spectral representation of the dry matter content in the tuber and a correspondingly better prediction. Another possible explanation is that the recording and averaging of multiple spectra across a moving potato may eliminate most of the contribution from local skin defects, such as scabs and scurfs common on potatoes [27]. In this study three replicates of each potato tuber were averaged before the calibration model were obtained. However, based on a PCA analysis of the replicates (data not shown) and the information in Fig. 4, no large replicate variance is seen. Hence, one replicate may be enough if the instrument is mounted above a conveyor belt. It should also be noted that the validation approach used in the current study, i.e. leave-one-out cross validation, often is regarded as an optimistic approach. Thus, for industrial applications additional data, based on independent test sets, should be added. However, in the present feasibility study, the validation approaches could be regarded as sufficient.

One of the most important aspects of on-line prediction of the dry matter content is speed. According to Brunt and Drost [28], the starch industry can receive up to 250,000 kg, or 10 truckloads, of potatoes per hour during peak season. The speed of the raw material flow, of course, depends on the number of conveyor belts used to handle the incoming raw material. It is unlikely that this amount can be handled by one single conveyor belt, and multiple instruments may be required to ensure good coverage. Brunt and co-workers made a prototype machine for prediction of starch and dry matter content in potatoes [29]. They briefly investigated the use of NIR for dry matter content prediction, but in the end traditional gravimetric prediction of the dry matter content was used. The authors stated that 10 samples per hour would suffice for their needs, each sample containing 3–5 kg. To sample one sample (5 kg) for each 10,000 kg is also common when using the gravimetric method for determining dry matter content. This equals 25 samples per hour (total of 125 kg of tubers), if calculating with the before mentioned amounts of potato. The conveyor belt in the current study was moving at 15 cm/s during the on-line measurements. Based on the number of spectra obtained from each potato tuber (approx. 15 spectra per tuber) it seems obvious that the speed can be increased. The prediction performance was largely maintained, provided that spectra used for dry matter content are samples from the entire length of the tuber. If increasing the speed to 25 or 30 cm/s the system would be able to measure nearly 300 individual tubers (with size of approximately 50 mm) per minute. This should be well within 10 samples per hour, and maybe also as much as 25 samples, allowing for different sampling regimes. Hence, the speed of the system demonstrated in the current study should have the capabilities to be incorporated in an on-line application. It is, however, expected that the current approach could be used at significantly elevated conveyor belt speed.

Robustness and variety independence are two key features in order to develop an industrial method for determination of dry matter content. The method used cannot be cultivar dependent or be affected by the skin color of the potato. A PCA analysis of average spectra from all on-line measurements is thus provided in Fig. 5. As can be seen, there seems to be a slight grouping along PC2. However, dry matter content and cultivar is slightly confounded, as shown in Table 1. Labeling the samples in the PCA plot with the corresponding values for dry matter content, reveals that the dry matter content is explaining the variation seen along PC2. This, rather than cultivar dependent differences, seems to be a more likely explanation for the slight grouping seen in Fig. 5. The PCA also indicates that the measurements are unaffected by the skin color. The two red colored cultivars (Asterix and Bruse) do not differ from the cultivars with yellow skin (Fakse, Folva, Mandelpotet, Saturna and Sava) along any of the two first PCs. This could also be related to the fact that the skin of the potatoes is only about 0.25 mm thick [19], and the interactance instrument sends light up to 20 mm into an unpeeled potato [4]. Hence, the skin should give an insignificant contribution to the spectra in this configuration. Noticeable differences due to flesh color was not

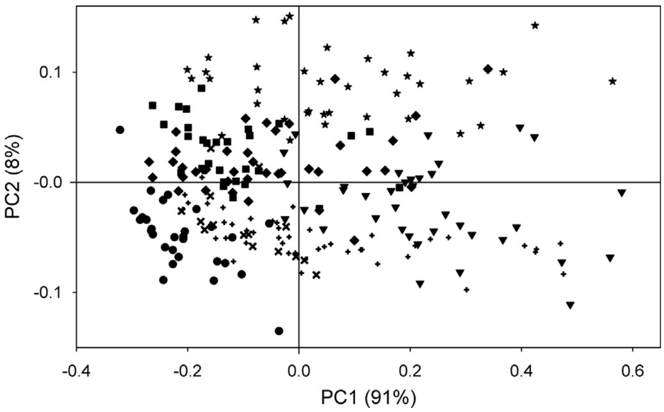

Fig. 5. a) A PCA analysis of the averaged spectra from the on-line measurements showed no clear grouping of the cultivars, Asterix (●), Bruse (★), Fakse (▾), Folva (**x**), Mandel (■), Saturna (◆) and Sava (+). PC1 explains 92% and PC2 explains 8% of the variance.

seen, and is also unlikely, since all cultivars used had yellow or light yellow flesh color.

4. Conclusion

The current study shows that the use of a high speed NIR interactance instrument with a low resolution spectrophotometer measuring 15 wavelengths is a feasible approach for on-line prediction of dry matter content in potatoes. The extraction of spectra from the background could be fully automated, and the dry matter content could be rapidly and accurately predicted on-line for individual potatoes. The model obtained from on-line measurements was significantly better than the model obtained from the off-line non-contact configuration and as good as the ones obtained from measurements in the off-line contact configuration. This was ascribed to a more representative sampling when measuring in the on-line configuration. Even dry matter gradients along the longitudinal axis of individual potatoes are reflected in the NIR spectra. The current measurement configuration only allows for measurement of one row of single potatoes, but it is expected that further instrumental development could increase expected sample throughput. The development of a user friendly instrument with the necessary hardware adapted to suit industrial environments is the natural next step in this development.

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