Determination of outer skin in dry onions by hyperspectral imaging spectroscopy and chemometrics

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The scope of this work is to propose a method based on near infrared hyperspectral imaging to automatically sort different parts of onions (dry peel, outer skin and onion bulbs) produced during specific industrial processes. For this purpose, two procedures have been developed; one is based on computation of the spectral area related to the organic sulphur band and the second one based on the discriminant chemometric tool PLS-DA. Both procedures have been compared by repeated measurements on artificial mixtures of dry peel and onions. This comparison indicated that PLS-DA produced the most accurate values while the study of spectral area seems to have the best repeatability. The PLS-DA procedure was then applied to several samples of mixed dried onions to compare the results with reference values obtained by manual counting. Based on the measurement repeatability, the stability of the results and the small differences between the reference and predicted values, this study has demonstrated the ability of near infrared hyperspectral imaging to identify and quantify the different parts of dry onions in mixtures.

Introduction

nions are one of the most common types of edible bulbs and vegetables consumed in the world. Onions come in a variety of shapes, sizes and flavour intensities and can be dried for storage purposes and later cooked into any recipe that calls for fresh onions, such as soups, sauces, beans and casseroles. Dry onions can be red, white or yellow in colour and are harvested when the bulb has reached maturity, the shoots have died and the onions are left with a papery covering. As these onions dry, pigments in the skin determine colour, which varies depending on variety. Some types of dry onions, such as Vidalias and Walla Wallas, are harvested very early and have a thinner skin and a higher concentration of sugar than other dry onions. These onions have such a sweet, mild flavour so that they are often eaten raw. Shallots are smaller, milder in flavour and tend to have two to three individual bulbs that grow next to each other under their papery outer skin. This outer skin is usually thrown away (more than 500,000 tons in the European Union each year) or processed and dried together with the onion bulb which may subsequently create problems in the preparation of specific recipes. Usually, in the preparation step, the product undergoes a high-temperature cooking that can considerably change the texture of plant tissues due to changes in the fibre components and result in the onions becoming soft.¹ The main problem, however, is that some pieces of onions, i.e. the peel outer skin, cannot be softened and

have a plastic appearance which causes many customer complaints regarding the final product. There is, then, a need to separate the different parts of onions produced during the industrial process, not only for the improvement of quality in the final prepared food but also for the valorisation of these products as this would enable them to be individually used as a source of functional compounds to be added to other foodstuffs.² Studies have shown that the brown skin and external layers are rich in fibre and phenolic compounds which have perceived benefits for human health. The dietary fibre could help to reduce the risk of developing cardiovascular or gastrointestinal diseases. Phenolic compounds, especially flavonoids, help to prevent coronary disease and have anti-carcinogenic properties. High levels of these compounds in the dry skin and the outer layers of the bulbs also give them high antioxidant capacity. The addition of value to these vegetable by-products is one of the main objectives of industry today and requires the development of novel non-destructive measurement tools allowing online applications in grading and process control systems as well as fast screening of quality. For this, techniques based on the use of vibrational spectroscopy such as near infrared (NIR) spectroscopy have gained industrial importance in recent years. This technique allows nearly instantaneous, non-destructive, noninvasive measurement with minimal sample preparation and collection of continuous real-time data. In the case of onion wastes. only few studies have examined the use of NIR spectroscopy to enhance the potential usefulness of onions by facilitating the identification of several functional products with different applications in the food industry. These reports have been mainly based on monitoring of alcoholic fermentation of onion juice by NIR spectroscopy² and the conversion of onion waste to onion vinegar.³ Recent advances in the spectroscopic field have allowed the extension of NIR spectroscopy from a point measurement to collection of an image (digital imaging) containing thousands of points, useful for exploring the spatial composition of samples, by hyperspectral imaging. This technology enables spectral as well as spatial information to be recorded simultaneously in a three-dimensional hyperspectral image (or hypercube) in which the two first dimensions provide spatial information with the third contributing spectral data. The main advantage of this technique is that, in addition to the identification and quantification of chemical constituents, their spatial location can be examined as well.⁴

In this study, the overall objective was to develop a protocol based on NIR hyperspectral imaging and chemometrics for accurate and objective detection of onion waste specifically in terms of dry skin. A successful outcome will help to add value to this dry outer layer skin as a food ingredient rich in specific, health-enhancing compounds. Specific objectives were to extract spectral information, identify optimal wavelengths and apply multivariate image analysis to identify and differentiate onion waste from onion bulb in dried

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Figure 1. RGB images of dry onions (left) and dry onion skin (right) fragments used for building the spectral library.



Figure 2. NIR hyperspectral images of dry onion flesh (left) and dry onion skin (right) fragments.

samples. An additional goal was to develop a complete image processing procedure to interpret the results obtained from the multivariate analysis.

Material and methods

For this work, six samples of dried onions obtained from a single supplier were studied. These products are commonly used as an ingredient in the finished product "Flemish stew". Once the final product has been produced, dry skin can be misinterpreted as plastic pieces and lead to complaints from customers. Usually, after internal checking, no plastic can be found but only dry onion skin, which is not normally mentioned in the product data sheet information.

For this work, a NIR hyperspectral line scan (also called push-broom imaging system) combined with a conveyor belt (BurgerMetrics SIA, Riga, Latvia) has been used. The system is equipped with a lighting device that illuminates the sample and the reflected light is collected by a twodimensional Focal Plane Array (FPA). Each acquired image consists of 320-pixel lines acquired with 209 wavelength channels in the range 1100-2400 nm with a spectral resolution of 6.3 nm. Thirty-two scans per image were averaged.⁵ Spectral acquisition was done with HyperPro software (Burger-Metrics SIA, Riga, Latvia) and the complete data analysis was performed using Matlab software (The MathWorks, Inc., Natick, MA, USA) together with the associated PLS and MIA toolboxes (Eigenvector Research, Inc., Wenatchee, WA, USA).

Results

Before starting, dry onion skin and dry onion flesh were first manually sorted (Figure 1) and weighed, then measured using the NIR hyperspectral imaging system (Figure 2). One image was collected from each pure ingredient to create a spectral library from which only 100 spectra (50 of dry onion bulb and 50 of dry skin) were selected for the construction of a discriminant model allowing differentiation of dry peel skin from dry onion bulbs.

For this purpose, two procedures were developed. The first one was based on the computation of the spectral area attributed to the sulphur compound; these are a subclass of organic compounds and are known for their variable occurrence concentrations and unusual properties. The second procedure was based on the discriminant chemometric tool PLS-DA.

Procedure based on specific spectral area

A NIR absorption band around 1740nm contains useful information related to sulphur compounds and corresponds to the 1st overtone vibration from –SH stretching.⁶

Onions are rich in sulphur compounds and, for this reason, once the images were acquired, a protocol was established to compute, for each pixel composing an onion fragment in the images, the area under this spectral band ("band area") and above the straight line connecting the two points on the NIR spectrum defining the sulphur compounds band (Figure 3).

The "band area" procedure developed consisted of different steps. In a first step, a principal component analysis (PCA) was applied to the image allowing a reduction of the space into new variables (principal components) that explain the maximum variability in the data set. The image reconstructed using only the first principal component explains mainly lighting effect interferences and provided a good contrast between the different onion fragments and the background. This principal component was used to highlight the different onion fragments



Figure 3. Estimation of the band area attributed to sulphur compounds (areas under the curves) in dry onion flesh and dry onion skin.

from the rest of the image using the intensity value associated with each pixel. Once the onion fragments have been isolated, in the second step of this protocol, individual spectra were processed in order to compute the area under the selected "sulphur compounds band". The limits of the "sulphur compounds band" were defined by the two minima observed in the NIR spectra around 1650 nm and 1900 nm, respectively. These two minima were automatically computed for each individual spectrum (pixel) and implemented in the computation of the "organosulphur band" area.

Figure 3 indicates that both dry onion flesh and dry onion skin fragments contain sulphur compounds. However, the dry onion flesh has a higher band intensity in the region attributed to sulphur compounds than that of the dry onion skin. In a second step, the difference of band intensity was used to sort the onion fragments by setting a threshold representative of the maximum absorbance value in the 1650-1900 nm region of the dry onion skin spectra. To do so, a preliminary calibration set has been built with dry onion skins and the 95th percentile of "sulphur compound band area" was computed amongst all pixels of the dry onion skin fragments contained in the image; this represents the value below which 95% of the pixels may be found.



Figure 4. Calibration set for classification of dry onion skin and dry onion flesh fragments.



Figure 5. Sorting of dry onion skin and dry onion flesh by PLS-DA.

Then, this value was used as a threshold for the classification of spectra from pixels taken from images of new samples. The last step of the "band area" procedure was the attribution of a prediction class (skin or flesh) to each pixel of dry onion fragments in new images. Figure 4 shows, as an example, the results obtained when the threshold was applied to the calibration set. The prediction of dry onion flesh pixels appear in dark orange and the dry onion skin pixels appear in yellow. From the image, it can be observed that all dry flesh fragments were correctly sorted and only one dry skin fragment seems ambiguous in its classification since it was mostly sorted as flesh. This unexpected result could be explained by the fact that it was difficult to manually or visually distinguish skin and flesh fragments when sorting samples, which can result in a misclassification even within the calibration set.

Procedure based on the chemometric tool PLS-DA

A second procedure based on the chemometric multivariate discrimination technique PLS-DA (Partial Least Squares Discriminant Analysis) has been applied and compared to the results obtained with the "band area" procedure. PLS-DA allowed the construction of a discriminant model between spectra issued from images of fragments from dry onion flesh and dry onion skin. PLS-DA is a method which is particularly useful when a set of dependent variables need to be predicted from a large set of explanatory variables (i.e. absorbance at different wavelengths) that can be strongly inter-correlated. In practice, there are two phases in the PLS-DA, the construction of the discriminant model and its subsequent validation.

To build the PLS-DA model, the same images as in the previous procedure were used (see Figure 4). The upper part of the image was selected to create the library used to calibrate the PLS-DA and then the entire image was used to validate the model. The library is composed of three classes; the first consists of spectra from dry onion flesh parts, the second of spectra from dry onion skin fragments and the last class contains spectra from the background. Figure 5 shows the three classes the dry onion flesh is in red, the dry onion skin in blue and the background in green.

A conversion factor from pixel to weight has been obtained to estimate the mass of dry onion skin and dry onion flesh. To do so, 202.8 mg of dry onion flesh and 202.8 mg of dry onion skin fragments were weighed. These samples were predicted by the PLS-DA model and the results gave, respectively, 1665 pixels of dry onion flesh and 10,737 pixels of dry onion skin fragments. By dividing each weight (202.8 mg) by the respective number of pixels, we obtained 0.0188 as the conversion factor for dry onion skin and 0.1218 for dry onion flesh.

To validate these conversion factors, two samples were measured six times under the same conditions. The first sample of 405.6 mg was composed of 202.8 mg of dry onion flesh fragments (corresponding to five pieces) and 202.8 mg of dry skin fragments (corresponding to 21 pieces) while the second sample of 728.8 mg contained

Table 1. Validation of the conversion factors from pixel to weight.

	First validation			Second validation		
	Predicted values			Predicted values		
	Reference values	Band area	PLS-DA	Reference values	Band area	PLS-DA
Mass of dry onion flesh (mg)	202.08	252.3 (±10.54)	228.01 (±14.77)	689.3	600.76 (±12.74)	615.01 (±33.40)
Mass of dry onion skin (mg)	202.08	201.3 (±5.63)	216.55 (±12.47)	39.5	26.4 (±1.23)	28.25 (±2.17)
Mass percent- age of dry onion flesh (g/100g)	50	55.61 (±0.7)	51.29 (±1.19)	94.58	95.8 (±0.19)	95.61 (±0.51)
Mass percent- age of dry onion skin (g/100g)	50	44.39 (±0.7)	48.71 (±1.19)	5.42	4.21 (±0.19)	4.39 (±0.51)

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39.5 mg of dry skin fragments (corresponding to five pieces) and 689.3 mg of dry onion flesh fragments (corresponding to 13 pieces). The conversion factors were then applied to all these images and the results are presented in Table 1.

Table 1 shows that the results obtained with the band area procedure systematically exhibited the smallest standard deviation which denotes a better repeatability. However, the predictions obtained with the PLS-DA model were the closest to the reference values (i.e. manual counting). For this reason, the PLS-DA model was applied to the six available commercial mixture samples obtained from the supplier.

Table 2 shows the PLS-DA predictions and reference values (manual counting) for the six samples. From this table it can be concluded that hyperspectral imaging produced results with less variability than manual counting. The measurement repeatability, the stability of the results and the small differences between the reference values and the predicted values demonstrated that it is possible to use NIR hyperspectral imaging to identify and quantify dry onion flesh and dry onion skin fragments in a mixture containing both.

Conclusions

In this paper we have described a preliminary study for the development of an automatic procedure based on the spectral band related to sulphur compounds which can be used for discrimination and quantification of dry onion skin and onion flesh fragments. The results obtained from this tentative study have been compared to the results obtained with a PLS-DA based procedure. Results indicated that, despite
 Table 2. Comparison of the PLS-DA prediction to the reference values (manual counting) for six commercial samples.

	Dry on	ion flesh	Dry onion skin		
Sample ID	Manual counting (g/100g)	Hyperspectral imaging (g/100g)	Manual counting (g/100g)	Hyperspectral imaging (g/100g)	
А	88.5	91.16	11.5	8.84	
В	92.7	92.76	7.3	7.24	
С	93.3	93.79	6.7	6.21	
D	85.6	93.65	14.4	6.35	
E	91.6	94.81	8.4	5.19	
F	91.7	91.98	8.3	8.02	
Mean	90.6	93.03	9.4	6.98	
Standard deviation	2.94	1.33	2.94	1.33	

the better repeatability of the "band area" procedure, the PLS-DA model procedure provided more accurate analyses. Performance accuracy of the PLS-DA model has also been confirmed by the analysis of several real samples from a supplier for which manual sorting has also been performed. However, the results obtained in the present study clearly demonstrated that the "band area" procedure has the potential to be a useful analytical method and deserves to be explored in greater depth. In addition, both PLS-DA and "band area" procedures could be easily implemented in companies for online detection of dry onion skins, which are particularly undesired in prepared foods.

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