

Discrimination of durum wheat products for quality control

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Introduction

Industrial hard wheat milling is a complex procedure, involving many operations (Figure 1). The grain is first cleaned and conditioned by dampening and then is submitted to the action of break rollers. Break rollers are able to grind the grain and to separate the endosperm from the hulls, with a minimal production of fine products. Plansifters, consisting of a series of stirred sieves, make it possible to classify the products according to their granulometry. The sieved

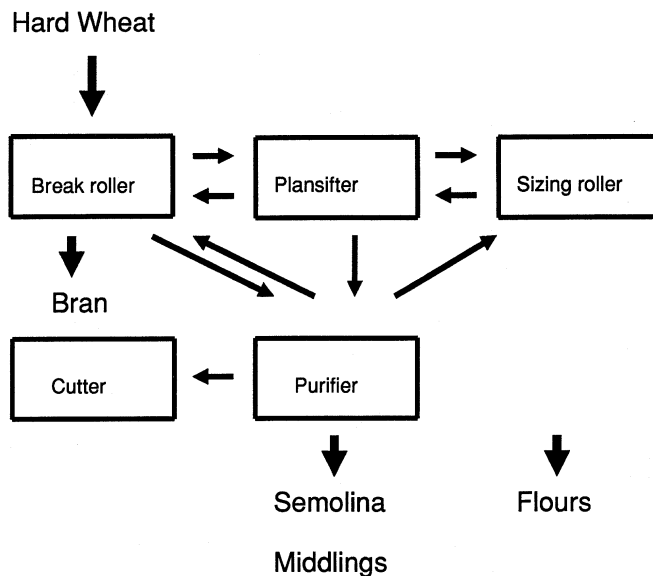


Figure 1. Diagram of hard wheat milling.

fractions obtained from plansifters are directed to purifiers where sieving and air-classification are combined to separate fractions of endosperm from outlayers parts. Semolinas of different grades are obtained from the purifiers. The coarser fractions which were not separated by sieving or air classification are ground again by sizing rollers and reintroduced into the production line.

For the production of semolina, used in the pasta industry, it can be necessary to reduce the granulometry of the obtained semolinas. This can be achieved by other roll grinders called “cutters”.

In the present work, we investigated the application of near infrared (NIR) spectroscopy for the control of industrial durum wheat milling and the quality assessment of the end products. As the milling process produced many types of end products it was decided not to develop calibration equations for specific components of each of them but rather to adopt a more global approach in which all the NIR spectra were gathered in a single spectral collection.

Material and methods

Sample collection

The experiments were conducted as a part of a plant selection program. The objective of this program was to study the relative importance of growing conditions and variety on the grain behaviour during milling. Six French varieties of *durum* wheat (1; *Agridur*; 2; *Arcour*; 3; *Ardente*; 4; *Capdur*; 5; *Exodur* and 6; *Primadur*) were grown in four agricultural conditions, namely *N1*, *N2*, *W1* and *W2*.

- *N1* and *N2* corresponded to two levels of nitrogen supplies (*N1*: Low; *N2*: High) at a location in Auzeville (France).
- *W1* and *W2* defined 2 levels of water supplies (*W1*: water stress, *W2* normal supply) at a location in Mauguio (France).

The 24 batches of wheat were processed in an experimental semolina mill which simulated an industrial process. The milling diagram of this pilot plant has been described previously by Houliaropoulos *et al.*¹

The process made it possible to obtain 16 end products:

- six kinds of semolinas differing by their “purity” (degree of contamination of the endosperm by outer cell-walls) coded from *S1* to *S6*, plus the blend of these semolinas (*ST*).
- four flours collected after the break rollers coded *B1* to *B4*.
- four flours collected after the reduction rolls (*R1* to *R4*)
- one sample of middling (*MI*).

According to the milling diagram, the semolinas could be graded on the basis of their purities into four qualitative groups: *S1* with *S3*; *S4* alone; *S2* with *S5* and *S6* alone.

The NIR spectra of the end products and of the grains were recorded on a NIR spectrometer (Bran+Luebbe InfraAlyzer 500) in reflection mode, from 1100 to 2500 nm at intervals of 4 nm. The samples were not ground before spectral acquisition, with the exception of the grains which were ground in a laboratory mill (Cyclotec) fitted with a sieve having an aperture of 1 mm.

Data processing

Principal component analysis (PCA) was applied on the whole spectral data set (matrix of 408 × 351 data points) with no pre-treatment of the spectra.

Stepwise discriminant analysis (SDA) was performed on the scores of the previous PCA with a stepwise introduction of the components, according to Bertrand *et al.*²

Results

Principal component analyses

The PCA map of the two first factors (Figure 2) was found to be the most interesting. With no supervised learning, the spectra were partly grouped according to the nature of the corresponding samples. Most of the semolinas could be identified with only weak overlaps. The direction from semolinas 6 to semolinas 1–3 is representative of their difference in purity. On the contrary, the flours were not well separated. A part of the separation, associated with the first component, was obtained from the variation in the general intensities of the spectra. It is well known that this intensity is related to the particle size of the studied samples. The second factor seemed to be representative of a variation in the chemical composition of the samples and in their proportion of starch.

Surprisingly, the growing location of the wheat (*N* in comparison with *W*) caused marked differences in the spectra for almost all the end products. On the contrary, neither the effect of nitrogen supply (*N1* in comparison with *N2*) nor that of water (*W1* and *W2*) could be identified.

A sub-collection, including only the spectra of grains (*GR*) and those of semolinas *ST*, was prepared, in order to examine the relationship between the raw materials and the transformed products. A second PCA was applied on this collection. The map of the two first factors is shown in Figure 3. As the granulometries were different, the first component obviously separated the semolinas from the grains. For the second component, a clear relationship between the spectra of grains and those of semolinas *ST* was visible. In order to emphasise this relationship, a line was drawn between the point corresponding to a sample of grain and that of the semolina obtained

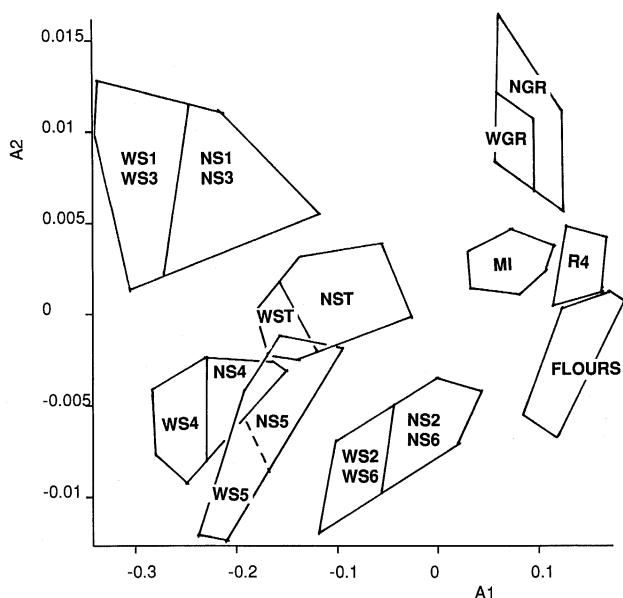


Figure 2. Principal component analysis on the whole spectral collection. (Plan 1–2) Only the areas occupied by each kind of products are shown. (*W*, *N*: growing locations of the processed wheat, *S1* ... *S6*, *ST*: Semolinas, *R4*: flour #4 after the reduction rolls, *Flours*: other flours, *MI*: middlings, *GR*: grains.).

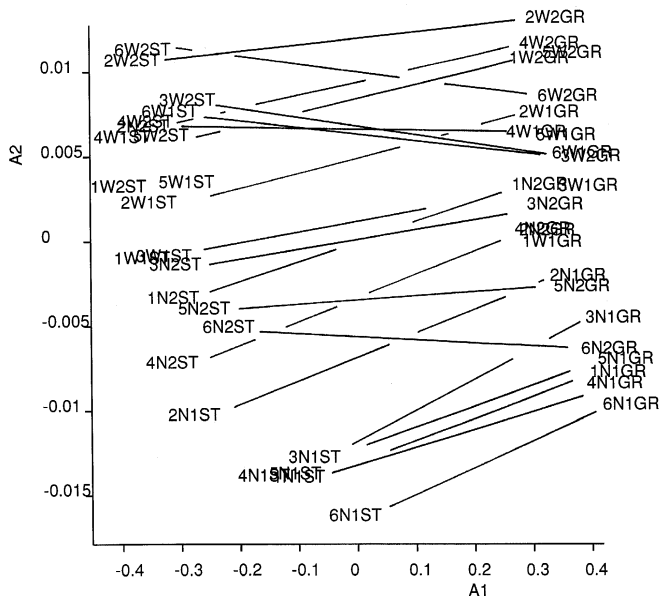


Figure 3. Principal component analysis of the spectra of grains and ST. (Plan 1–2) Code (see Materials and methods): First letter: variety, Second and third: agronomic condition, Fourth and fifth: Semolina (ST) or grain (GR). The grain and its corresponding semolina ST are joined by a straight line.

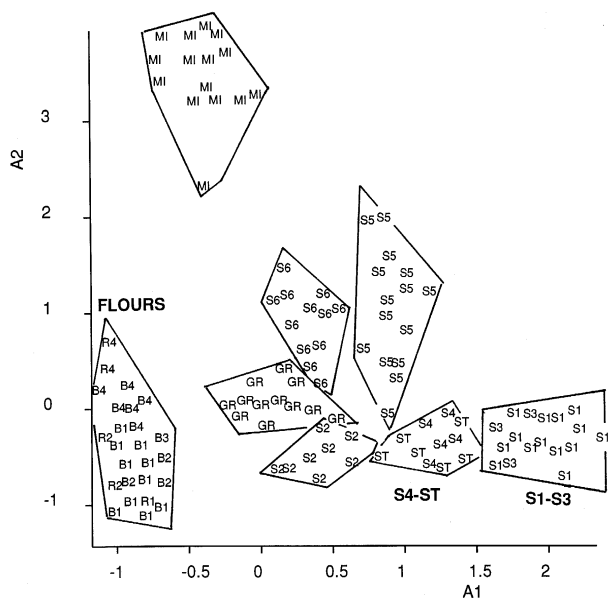


Figure 4. Factorial map of discriminant analysis. (Plan 1–2) The overlapping points are not represented but do not change the interpretation of the map. (Code: see Material and methods *Flours*: samples B1 ... B4, R1 ... R4).

Table 1. Classification of semolinas by discriminant analysis.

	Predicted						
	S1	S2	S3	S4	S5	S6	ST
Actual	S1	16	4				4
	S2		24				
	S3	3		21			1
	S4			24			
	S5				23	1	
	S6					24	
	ST					1	23

from its processing. The grains and the corresponding semolinas, *ST*, were ranked in comparable order according to the second factor. This result showed that, even after a complex milling procedure, the spectra of semolinas contained chemical information which was specific for the grain from which they were obtained.

Stepwise discriminant analysis

For discriminating the nature of the samples (16 kinds of end products plus the corresponding grains) from their NIR spectra, SDA was applied on the whole spectral collection. By introducing

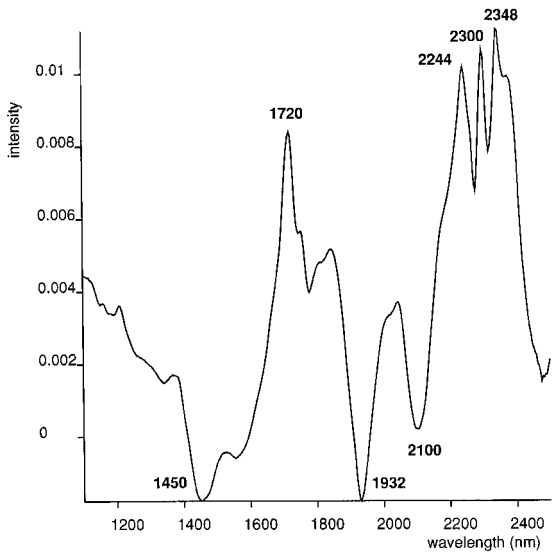


Figure 5. Second spectral profile of discriminant analysis. (Numerical values: wavelengths in nanometers).

eight factors of the previous PCA, it was possible to obtain about 80 percent of correct classification in the 17 qualitative groups, with some products having no misclassified samples (*S2, S4, S6, MI, GR*). On the contrary, most of the flours (*B1 to B4* and *R1 to R4*) presented many incorrect identifications and were often confused with each other. Among the semolinas (Table 1) the classifications were generally relevant and the confusions were generally observed only between semolinas of the same purity (for example *S1* with *S3*). Some of these misclassifications, such as *S1* or *S3* with *ST*, were less acceptable for grading the products industrially. The map of discrimination (Figure 4) shows that the spectra could be mainly discriminated according to two factors. The first one was again representative of particle size (from fine to coarse products according to the value of score 1). The second one was characteristic of chemical information. The corresponding spectral pattern is shown in Figure 5. It shows the opposition of negative spectral bands associated with starch at 1450 or 2100 nm to positive bands representative of C–H or C=H groups at 1720, 2300 or 2348 nm. It should be noted that almost exactly the same spectral pattern was previously obtained for a similar spectral collection.³

Conclusion

NIR spectroscopy seems to be a relevant method for the control of the milling process. As the assessment of complex calibrations is not required, the global approach which was adopted here is inexpensive and requires less time than the more classical procedures, especially when the end products are numerous. Much useful information can be extracted from NIR spectra. In the present case, the relationship between the growing location of wheat and its behaviour during milling was clearly emphasised. For each of the studies, the extracted spectral patterns were often very similar. This similarity merits further consideration, both for developing more universal methods of prediction and for a better understanding of the NIR spectroscopy of natural food products.

Acknowledgements

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