Chemometrics for the evaluation of white pudding ageing on the basis of near infrared spectroscopy

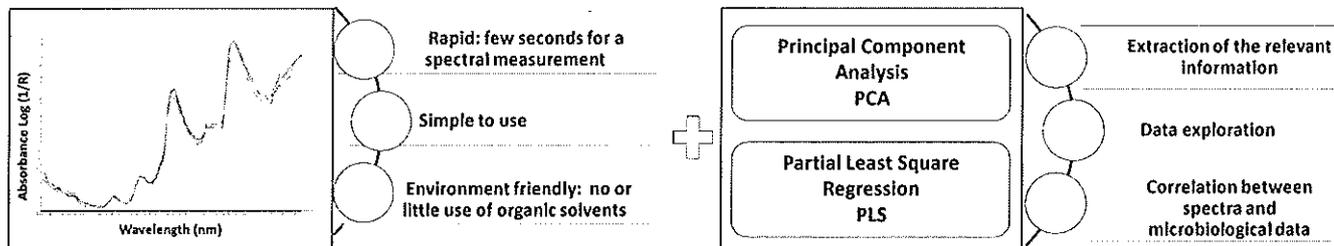O. Abbas*[1], Y. Adolphe[2], J.A. Fernández Pierna[1], A. Clinquart[2], G. Daube[2], V. Baeten[1], P. Dardenne[1]

[1]*Department of valorisation of agricultural products, Walloon Agricultural research centre, 24 Chaussée de Namur, Gembloux, Belgium*
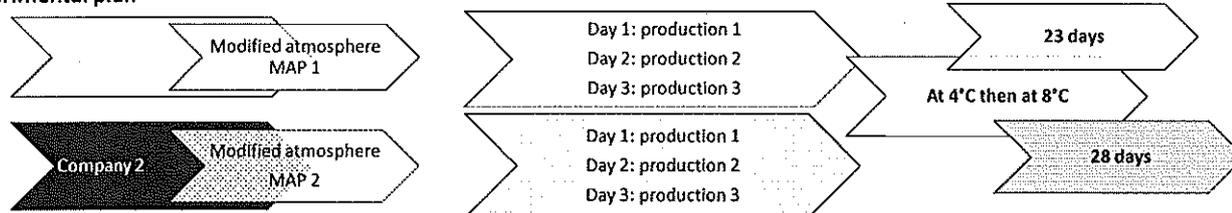[2]*Department of Food Science, University of Liège, Sart Tilman B43b, 4000 Liege, Belgium*
E-mail:

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The comprehension of the mechanisms leaded to food spoilage is necessary in order to bring more specific knowledge to the food producers about preparation and preservation. Researches made within the framework of the CONSALIM* project (financed by the Walloon Region) aim to adapt methods to food preservation requirements. The work presented here consists on the development and on-line application of rapid and non-destructive analytical techniques to reach this objective. The technology used in this work is the well known near infrared spectroscopy combined with Chemometric tools.

- Rapid: few seconds for a spectral measurement
- Simple to use
- Environment friendly: no or little use of organic solvents

Principal Component Analysis PCA

Partial Least Square Regression PLS

- Extraction of the relevant information
- Data exploration
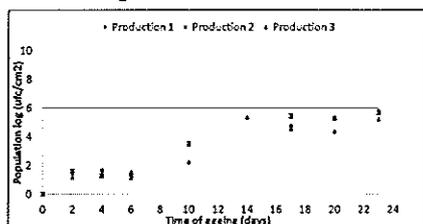- Correlation between spectra and microbiological data

To link the NIR technique and the acceptability state of the product, ageing tests of white pudding were carried out and the evolution of the growth of total flora was followed. The ageing was studied as presented below. Samples were analyzed by microbiological assays where Total mesophilic flora method was used (The count was performed at 30 ° C after 24 h of incubation, following ISO4833 norm), and by NIR spectroscopy where only the external face of the white pudding was analyzed.
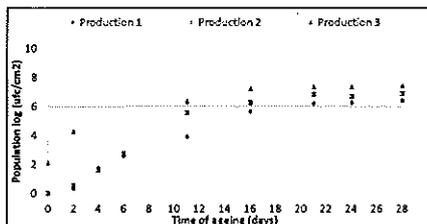
Experimental plan

Modified atmosphere MAP 1

Company 2 — Modified atmosphere MAP 2

Day 1: production 1
Day 2: production 2
Day 3: production 3

Day 1: production 1
Day 2: production 2
Day 3: production 3

23 days — At 4°C then at 8°C

28 days
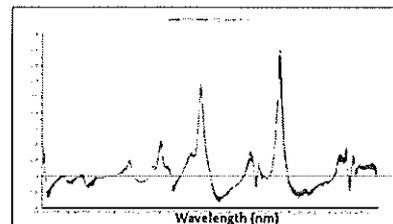
Microbiological results

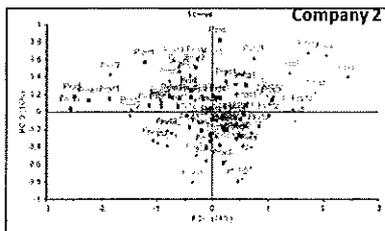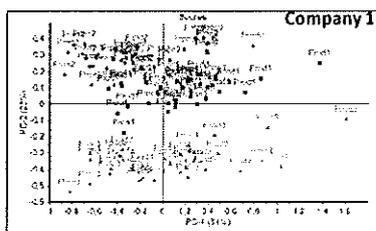*Evaluation of total flora of white pudding (company 1)*

Evaluation of total flora of white pudding (company 2)

Spectroscopic results

Example of NIR derivated collected spectra of white pudding aged

Distribution of samples of the three productions on the basis of their NIR spectra

Company 1

Company 2

PCA applied on spectra of companies (1) and (2) shows the variability that can exist in the produced white puddings.

Spectra were corrected by first derivative pre-treatment.

Graphs of PCA applied on NIR corrected spectra of the three productions of white pudding aged provided by companies 1 and 2

Correlation of spectroscopic and microbiological data: individual production sets of each company

Individual PLS models performances for the prediction of total flora values

Company	pre-treatment	Statistics values	Production 1	Production 2	Production 3
Company 1	SNV+ 1st derivative	R-Square	0,99	0,99	0,97
		RMSECV	0,55	0,78	1,03
		RMSEP	1,34	0,79	1,32
Company 2	SNV+ 1st derivative(1)	R-Square	0,93	0,93	0,99
	SNV(2)	RMSECV	0,91	1,29	0,55
	No pre-treatment(3)	RMSEP	1,87	1,21	1,6

PLS models developed on individual productions of each company show good performances for the prediction of the total flora of aged white puddings.
Calibration set = 24 spectra/production/company
Validation set = 12 spectra/production/company

Correlation of spectroscopic and microbiological data: Total production sets of each company

PLS models performances for the prediction of total flora values for all productions

Company	pre-treatment	R-Square	RMSECV	RMSEP
Company 1	1st derivative	0,81	0,95	1,06
Company 2	SNV	0,81	1,35	1,28

PLS models developed on total production of each company show lower performances for the prediction of the total flora than obtained when working on each production separately.
Calibration set =72spectra/production/company
Validation set = 36 spectra /production/company

Conclusion

Near infrared spectroscopy coupled to chemometric tools has a real potential for the analyses of fresh products. Results obtained on the evaluation of the ageing of white pudding are encouraging and studies will be continued in order to better estimate the total flora. Estimation of the total flora of one production on the basis of a model developed on the two other productions and/or the application of other chemometric tools like LS-SVM (Least Squares Support Vector Machines) regression are planned.

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