

The application of Fourier transform near infrared spectroscopy in the wine industry of South Africa

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Introduction

During wine production optimum yeast growth healthy alcohol fermentation rates are monitored by the amount of free amino nitrogen (FAN) present in the must.¹ The status of the malolactic fermentation (MLF) in Chardonnay wines must be monitored by determining the degree of conversion of malic to lactic acid.² Ethyl carbamate (EC), a suspected carcinogen, is mainly formed during the aging of wine under certain conditions and is restricted by legislation in some countries.³ It is, therefore, necessary to determine the EC content in wine. Currently these measurements are monitored using expensive, quantitative, time-consuming analytical methods. It would, however, be adequate to use a discriminate screening method as the samples need only to be classified as belonging to a certain class or having reached a specified cut-off point or not. Fourier transform near infrared (FT-NIR) spectroscopy can be used as a rapid method to discriminate between different must or wine samples. If the samples are spectroscopically dissimilar, spectral differences can be used.⁴ If the spectra are similar, sophisticated techniques such as soft independent modelling by class analogy (SIMCA) can be used. SIMCA takes into consideration both the variability of the spectra of interest and the differences between the spectra.⁴

Objective

The aim of this study was to apply SIMCA on FT-NIR spectra of must and wine to discriminate between the samples in terms of their FAN values, the status of the malolactic fermentation and the level of EC present.

Table 1. Respective classes into which the data were divided for each constituent.

Constituent	Class 1	Class 2	Class 3
FAN (mg N L ⁻¹)	1 – 800(<i>n</i> = 26)	800 – 2000(<i>n</i> = 71)	
MLF	Not started(<i>n</i> = 18)	Underway(<i>n</i> = 30)	Complete(<i>n</i> = 38)
EC (ppb)	0 – 10(<i>n</i> = 47)	10 – 15(<i>n</i> = 16)	> 15(<i>n</i> = 7)

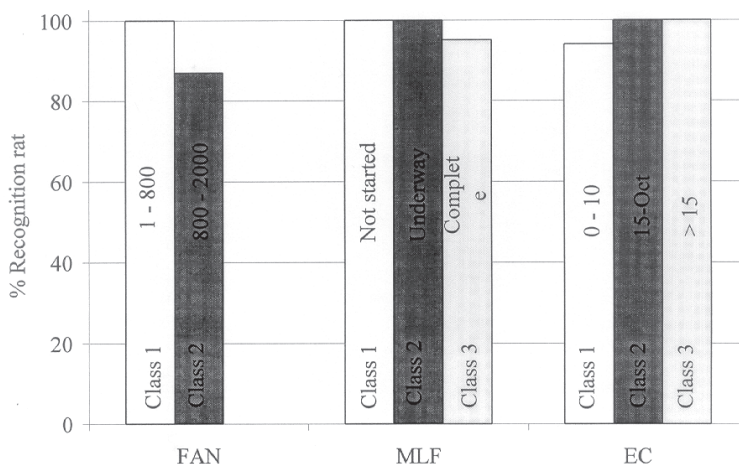


Figure 1. Graphic representation of SIMCA results.

Materials and methods

The FAN content of the must samples was determined spectrophotometrically by means of an auto-analyser.⁵ Determinations of the malic and lactic acid content of the wine samples were done by means of high-pressure liquid chromatography (HPLC),⁶ while the EC content of the wine samples was determined by means of gas chromatography with mass selective detection (GS/MS) according to the OIV method.⁷ Wine and must samples with known FAN ($n = 123$), malic acid ($n = 109$), lactic acid ($n = 103$) and EC ($n = 156$) values from the 1999 and 2000 harvest seasons were used. Optical absorption spectra for each sample were recorded using the FT-NIR Perkin-Elmer Spectrum IdentiCheck spectrophotometer over the range $10,000$ to 4000 cm^{-1} at 16 cm^{-1} resolution in a 0.5 mm path length quartz cuvette. Selected spectra for each constituent were divided into appropriate classes (Table 1) and models were built by performing principal component analysis (PCA) on 2^{nd} derivative spectra using QUANT+ software. SIMCA validation tests were performed on the models to determine the accuracy of the respective models.

Results and discussion

A summary of the results obtained with SIMCA are graphically illustrated in Figure 1. Efficient discrimination between samples has been achieved using SIMCA and FT-NIR can be used successfully as a powerful tool in screening spectroscopically similar samples.

The two models that were created for classes 1 and 2 for the FAN values (Table 1) showed good classification possibilities. The recognition rates were above 87% for both the data sets (Class 1 = 100%, Class 2 = 87%), indicating good separation of each class (Figure 1). Accurate classifications were possible with the three models that were created for the malolactic fermentation (Table 1). Recognition rates of above 95% were reported, indicating good classification of each class (Figure 1). Good classification possibilities were shown with the three models that were created for EC values (Table 2). The recognition rate columns reported 94% for Class 1 and 100% for Classes 2 and 3, respectively, indicating that excellent separation of each class had been achieved.

Conclusion

It would, therefore, be possible to replace expensive, time consuming quantitative analytical methods such as FAN, malic and lactic acid and EC determinations, if not completely, at least to some extent, with FT-NIR spectroscopy.

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