Classification of three-year old, unblended South African brandy with near infrared spectroscopy

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Introduction

Brandy is an unique alcoholic beverage produced through a double distillation process of brandy base (rebate) wine in a discontinuous fashion in copper kettles.[1,2] Maturation in French oak barrels for a minimum period of three years helps to produce a smooth, amber-coloured product which is pleasant to the palate and rich in bouquet and flavours. A considerable variety of amber-coloured beverages emerge from the maturation process, each with a different character, flavour and depth of colour.

The matured brandy is classified before blending in different styles based upon the sensory quality of the matured distillate, which can be described as a combination of fullness, softness and taste, as well as flavour intensity.[3] Blending is performed by adding and correcting constituents to obtain both uniformity within a brand name and a final product of established and recognised character.[1, 2]

In recent years NIRS has evolved into many specialised fields and the wine and distillation industries has kept up with the trend.[4-12] The expansion of the applications of near-infrared spectroscopy in the distilling (and wine) industry shows the potential to contribute to the optimisation of the processes involved and the improvement of quality control.

Near infrared spectroscopy (NIRS) could be used as an objective classification method to discriminate between the different brandy styles based on their chemical composition as it relates to their sensory quality. This would not only streamline the process, but also result in a more consistent classification procedure and product.

Materials and methods

Samples

Unblended three year-old brandy samples (191 samples from 3 seasons) were classified into four classes through sensory evaluation (20% alc/vol) by a trained panel. These four classes represented respectively four different brandy styles from the smoothest to the hardest, most “wooded”.

Spectral analyses

The samples were standardised to 43% alc/vol with distilled water before collection of the spectra. Near infrared spectra were recorded in transmittance mode at 2 nm intervals using a Perkin-Elmer Spectrum Identicheck^{TM} 2.0 FT-NIR system in the wavelength range between 700 and

2500 nm, with a 16 scan sequence at a resolution of 8 cm^{-1}. The liquid samples were presented in a 1 mm path length Quartz UV/VIS Spectroscopy cell.

Principal component analysis (PCA) and Soft independent modelling of class analogy (SIMCA) was performed using SIMCA-P software ver. 8.00 (Umetrics, Sweden) for qualitative analysis, i.e. classification of the samples according to class membership (Figure 1).

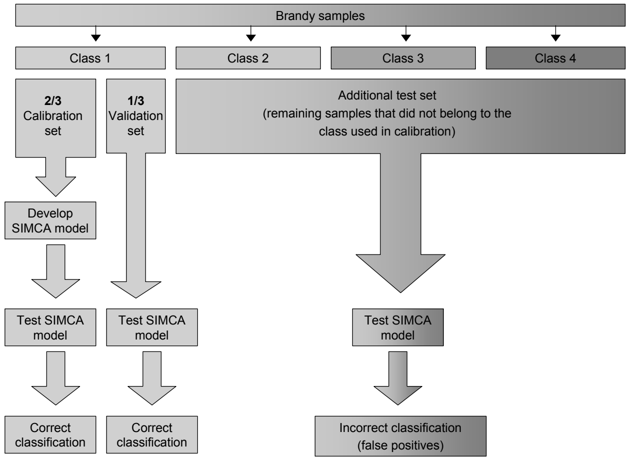

Figure 1. Schematic diagram of the SIMCA modelling and prediction testing

Results and Discussion

The absorption spectra obtained for the brandy samples are shown in Figure 2. Figure 3 shows the seasonal distribution of the samples as revealed through PCA of the absorption spectra.

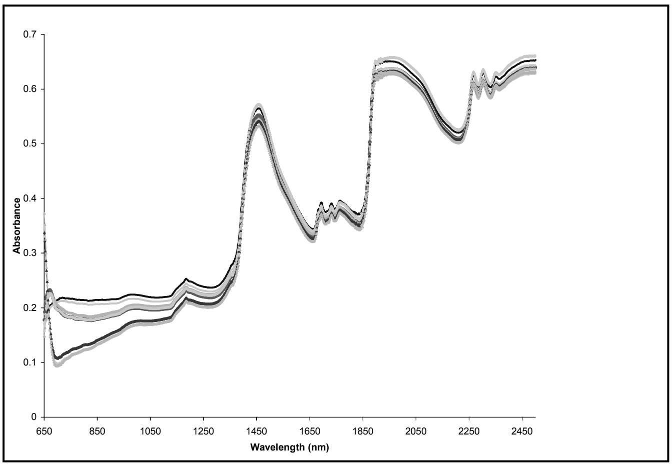

Figure 2. Absorption spectra of the brandy samples

The score plot indicated the need to separate the seasonal data sets and perform classification on each individual seasonal data set. SIMCA classification results obtained for the individual datasets of 1999, 2000 and 2001 are presented in Table 1.

Strong overlapping between samples of classes 2 and 3 in the 1999 and 2001 (Figure 4) data sets resulted in the poorer classification results obtained for these classes. This could be attributed to the slight sensory quality difference between the two classes and the complex sample matrix of the brandy with an array of compounds that all influence the sensory qualities of brandy in various ways. The smoothest and hardest classes (classes 1 and 4) showed the strongest clustering and predictive potential in all cases (Figure 4).

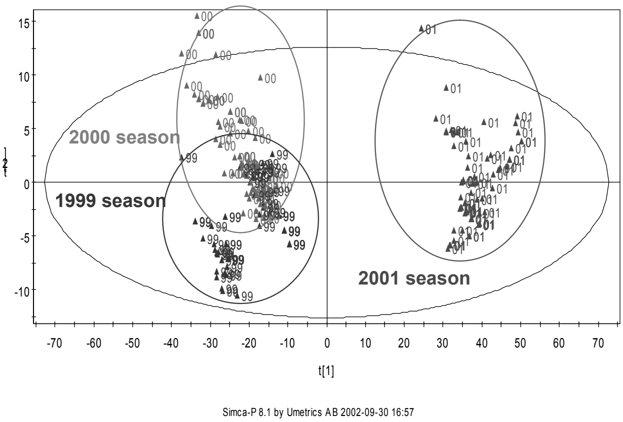

Figure 3. PCA score plot (PC1& PC2) showing the seasonal distribution of the entire data set.

Table 1. SIMCA classifications results of three-year old unblended brandy samples within seasonal data sets.

Classification		PC's	Correct classification (%) Cal set	Val set	Incorrect classification (%)
1999	Class 1	4	100	60	13.3
	Class 2	3	100	50	0
	Class 3	3	81.3	62.5	0
	Class 4	3	87.5	67.7	10.2
2000	Class 1	5	76.5	100	5.7
	Class 4	5	85.7	90.9	0
2001	Class 1	4	81.8	100	0
	Class 2	4	92.3	100	0
	Class 3	4	93.3	57.1	0
	Class 4	3	85.7	100	0

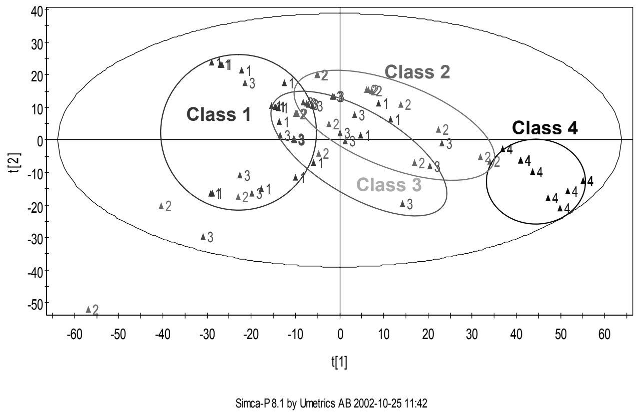

Figure 4. PCA score plot showing the class distribution of the 2001 data set.

Conclusions

Based on its classification power, NIRS combined with SIMCA appeared to be a promising tool when used in the analysis of unblended brandy. This technique could be employed to predict the season to which samples belonged season followed by the specific 'seasons' models to predict class membership. By adding new data sets from future seasons, a robust classification technique can be developed. Advances concerning automated liquid sample presentation of NIRS instrumentation could greatly enhance the spectral acquisition of the data and probably improve the predictive abilities of the modelling. Due to the slight differences between the NIRS absorbances of the samples and the variation induced through the subjective classification process, distinct clustering or grouping of the different classes could not be expected. NIRS and SIMCA offers a rapid and objective method to classify brandy samples according to on the basis of their classification status.

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