Non-invasive spectroscopic screening: A new approach to assessing damaged wines

Introduction

This case study presents an example of using BevScan's classification mode to screen and sort bottles of a red wine affected by variable bottle oxidation.

More general information about BevScan and about variable oxidation can be found in the following two AWRI fact sheets, available from www.awri.com.au

- **Introducing BevScan - a new tool for non-destructive wine analysis and classification**
- **In-bottle measurement of variable bottle oxidation**

Background

The Australian Wine Research Institute (AWRI) receives a number of enquiries each year from wine producers who have issues with the variability of their products due to inadequate storage conditions, insufficient care taken by distributors and retailers through the supply chain and variability during bottling. Sometimes, a large proportion of bottles are unsaleable due to high sulfur dioxide (SO_2) depletion, microbiological contamination, elevated colour development or oxidative sensory characteristics.

Summary

The AWRI, in conjunction with Angove Family Winemakers, used its BevScan™ technology to screen samples of a commercial red wine that were exhibiting random patterns of oxidation during storage and identify those bottles that had acceptable development characteristics.

A spectral classification model was built using samples of the wine that were exhibiting random patterns of oxidation. This calibration model was then used to screen approximately 700 cases of wine and identify those bottles that had acceptable development characteristics, allowing the mobilisation of stock for overseas markets.

Assessing the Problem

Six cases of the wine were supplied to the AWRI for spectral screening. All 72 samples were analysed using the BevScan™ instrument and spectral data was transferred to Unscrambler (CAMO, version 10.1) to undertake principal component analysis (PCA) and identify any differences/similarities among the samples. The spectral range was trimmed to 600-1000 nm for analysis and two groups of samples became apparent, as shown in the PCA plot below, with PC1 appearing to be related to the oxidised state of the wine. This appeared to offer an opportunity for discriminating between good and bad samples, non-destructively.

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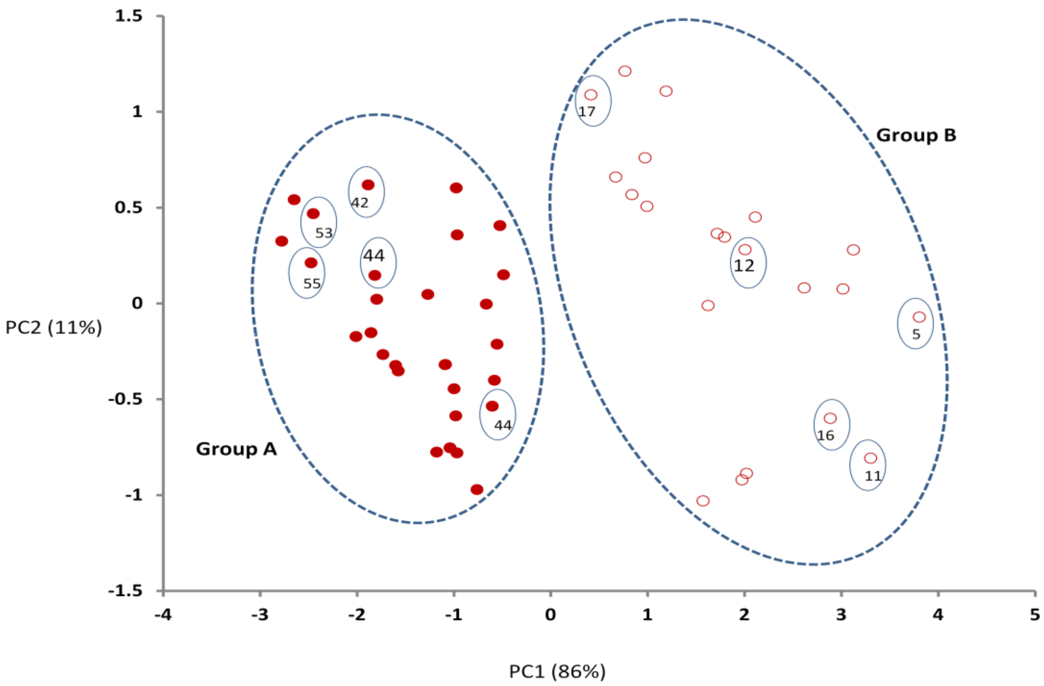

Figure 1. PCA plot based on spectral analysis of Angove wines. Each bottle was scanned once. Numbers in ellipses indicate the concentrations of total SO_2 (mg/L)

A random selection of ten bottles was collected, with five taken from each of the apparent groups, to assess the comparative degree of oxidation. Free and total SO_2 levels were measured, along with colour density and hue measurements. Analysis showed that the five samples with typical (expected) SO_2 levels and lower colour density and hue were all found in Group A, whilst the five samples showing significant SO_2 depletion and elevated colour levels were all in Group B.

Table 1. Chemical analysis data for ten randomly selected samples

Bottle Code	Colour density	Colour Hue	SO_2 free (mg/L)	SO_2 total (mg/L)
Group A				
e1	0.83	0.78	15	55
f1	0.82	0.77	15	53
f7	0.84	0.80	11	44
c3	0.85	0.80	10	42
d5	0.84	0.80	11	44
Group B				
c11	1.00	0.80	<4*	11
d3	1.04	0.82	<4	5
e6	0.98	0.80	<4	16
e10	0.95	0.80	<4	17
c12	0.96	0.82	<4	12

* Limit of detection by Flow Injection Analysis (FIA) method.

Building the classification model

In order to create a BevScan™ classification model for screening, the spectra from Group B were removed from the data-set and the remaining Group A spectra were used to describe acceptable spectral characteristics. An acceptable tolerance limit was set, so that samples could be classified correctly with approximately 95% confidence. Based on the PCA, the wavelength range was restricted to 600 to 1000 nm. This removed regions where absorbance levels were either in saturation or not contributing to the differences observed across the sample set.

Screening of damaged wine stock

In order to allow screening of the retained stock, the BevScan™ instrument was set up in the finished products warehouse at Angove's Renmark facility and all 716 cases were screened by Angove staff to identify acceptable bottles of wine using the BevScan™ classification model. Stock was segregated solely on this classification result.

The classification model allowed new samples, of unknown condition, to be screened non-destructively and provide a simple Pass/Fail response, which is defined by the characteristics of the acceptable set (Group A). The BevScan™ provides a 'score', which is an arbitrary determination of the mathematical similarity between the average spectral response of the samples used in developing the model and the sample being tested. A score of 10 or less indicates that the sample is spectrally similar to the samples in the classification model and a score of 1 indicates that the sample is spectrally identical to the average of the samples in the classification model.

Figure 2 shows the identification of an acceptable sample (c2), when the classification model is being applied to a sample of unknown condition.

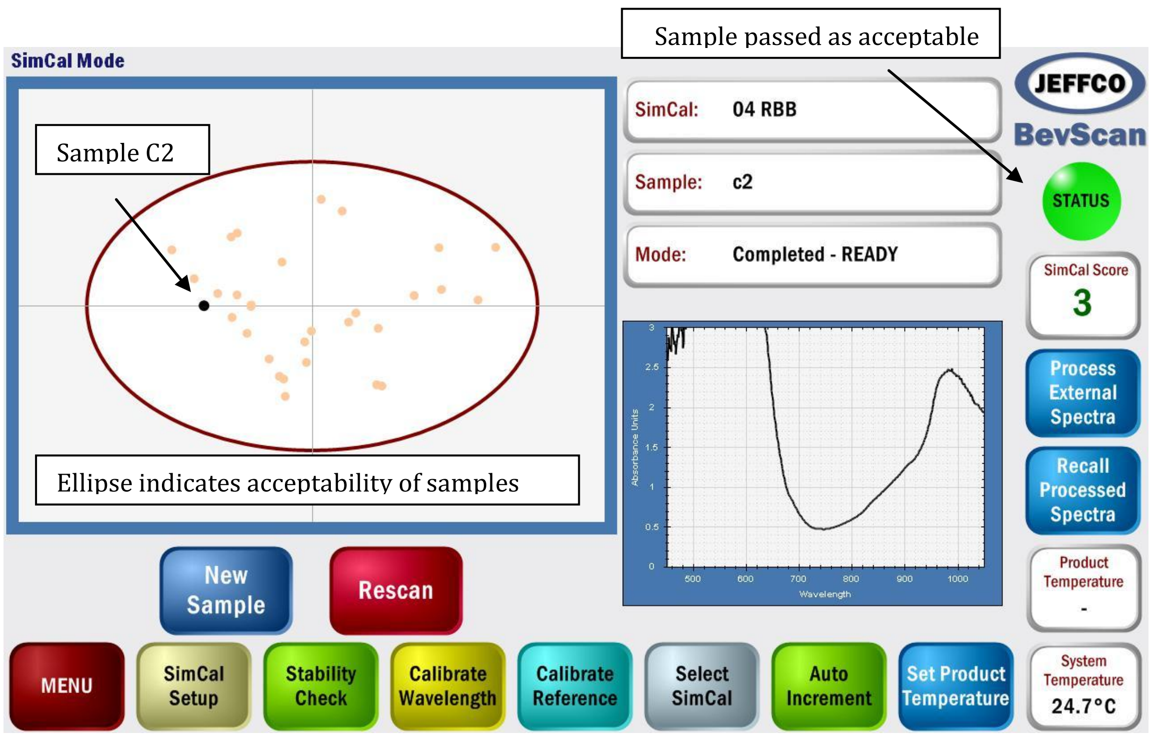

Figure 2. BevScan™ showing identification of an acceptable sample.

Of the 716 cases assessed, 375 cases of acceptable wine were accumulated and 341 cases were rejected.

Validation

Six cases of the rejected wine samples were sent to the AWRI for subsequent chemical analysis, to confirm the unacceptable (chemical) nature of these samples. A random selection of nine bottles was taken from the six cases, to assess the comparative degree of oxidation.

Free and total SO_2 levels were measured, along with colour density and hue measurements, as before. The nine samples were also re-screened in the AWRI laboratory using BevScan™, to determine if measurement temperature or bottle imperfections at Renmark had played a part in producing a higher incidence of false negatives.

Re-scanning of the samples at the AWRI confirmed that eight of the nine rejected samples were unacceptable. Only sample RBB 2 was deemed to be acceptable and only this sample showed typical (expected) SO_2 levels and lower colour density and hue (Table 2). Samples RBB 5, 3 and 7 all exhibited borderline acceptable chemical characteristics, but were deemed to be unacceptable when evaluated with the classification model (classification score >10).

Table 2. Chemical analysis data for nine randomly selected confirmation samples.

Bottle Code	Colour density	Colour Hue	SO_2 free (mg/L)	SO_2 total (mg/L)	Classification Score
RBB 1	1.01	0.84	< 4	7	100
RBB 9	1.01	0.85	< 4	< 4	100
RBB 8	1.01	0.84	< 4	6	100
RBB 4	1.01	0.84	< 4	6	100
RBB 6	0.99	0.83	< 4	10	53
RBB 5	0.92	0.82	5	25	25
RBB 3	0.90	0.81	7	30	22
RBB 7	0.89	0.81	8	33	12
RBB 2	0.85	0.80	12	45	7

Summary

BevScan™ has been shown to be a valuable tool for screening and classifying wine stock impacted by random patterns of oxidation non-destructively. By using this tool, Angove Family Winemakers has been able to mobilise otherwise worthless stock and supply their customers with wine which tastes the way the winemaker intended.

For additional information please contact us

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