Application Note 13
Identification of Distilled Spirits

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1. Introduction

A large problem for the distilled spirit industry is the time required for quality control. Typically, plant managers or other production people are taken from their daily job requirements to sniff samples to ensure the right product goes into the right bottle. A Cyranose 320 (C320) could help the plant managers by decreasing the amount of time they are required to sniff product. The goal of this experiment is to discriminate between 6 distilled spirits – Gin, Rum, Vodka, Whiskey, Whiskey Standard and Gin Standard and identify two unknown samples, 50/50 Mix Whiskey & Gin and Original formula Whiskey.

2. Experimental

Sample preparation:
2ml of 40 proof distilled spirits were added to 40ml screw top vials. 10 replicates of each sample were prepared. All samples were kept in a lab environment at ambient conditions. A heating plate was used to warm the samples to 75°F. This is consistent with the industry practice to hand warm the samples prior to sniffing. The key to the samples is in Table I below.

Table I. Key to Samples

Distilled spirit	Letter assigned to distilled spirit
Rum	A
Whiskey	B
Vodka	C
Gin	D
Whiskey standard	E
Gin standard	F
50/50 Mix Whiskey & Gin	G
Original formula Whiskey	H

Testing Conditions:
A Cyranose 320 with a 32-sensor array was used. All of the sensors reached a steady state response to the samples within the 15-second sample draw. The method settings are in Table II below. The training set was obtained by sampling vials randomly. Each sample was sampled once before the training set was built. The vials were sealed with a screw top lid and the lids were removed when sampling was in progress. Once the

training set was built, the C320 was used to identify the 2 unknown samples 50/50 Mix Whiskey & Gin and Original formula Whiskey.

Table II. Method Settings

C320 Parameters	Time	Pump Speed
Baseline Purge	10 seconds	Med
Sample Draw	15 seconds	Med
Sample Draw 2	0	N/A
Snout removal	0	N/A
1st Sample Gas Purge	0	N/A
1st Air Intake Purge	10	High
2nd Sample Gas Purge	30	High
2nd Air Intake Purge	0	N/A
Digital Filtering ON		
Substrate Temperature 42°C	All 32 sensors selected	Algorithm used – Canonical, Autoscale, Normalization - 1

Data handling:
Data was recorded with digital filter on. The sensor responses were calculated using the minimum of the resistance reading during the baseline purge and the maximum resistance reading during the vapor exposure, which is $(R_{max}-R_{min})/R_{min.}$ Canonical discriminant analysis (CDA), an algorithm for pattern recognition, with auto-scaling and 1-normalization was used for model-making and predictions.

3. Results:

The PCA and Canonical plot illustrate the discrimination of the samples (Figures 1 and 2). As shown in Figures 1 and 2, samples A (Rum) and C (Vodka) were not discriminated by the C320. Figure 3 shows the cross validation results. The cross validation results depict the inability to classify the A and C samples (Figure 3). The first table in Figure 3 shows that 7 of the 10 exposures trained to Class A were classified (identified) as Class A and the other three samples were classified as Class C using the CDA model. Similarly, 6 of the 10 exposures trained as Class C were classified (identified) as Class C and the other four samples were classified as Class A using the CDA model. All of the remaining exposures to Classes B, D, E and F were classified correctly in their respected Classes. This gives 88.3% correct cross validation. The second table in Figure 3 gives an indication of how far apart the 6 Classes are in the model. Interclass distances were in the range of 1.215 and 21.079, which indicates good discrimination among four of the six different samples. Class A and Class C has the smallest interclass distance of 1.215, which explains the reason for the mis-classification described above during cross validation. The small interclass distance, the lack of

discrimination in the PCA and Canonical plots and the cross validation table indicate the lack of discrimination between Class A and Class C. The remaining interclass distances ranging from 7.093 to 21.079 indicate good discrimination.

Refer to Table III below. The trained C320 was used to identify the unknowns. Three predictions of G (50/50 Mix Whiskey & Gin) and three predictions of H (Original formula Whiskey). The G sample always predicted as "Unidentifiable sample" which was perfect since it was a combination of 50/50 Mix Whiskey & Gin and we did not train to it. The H sample (Original formula Whiskey) predicted as E (Whiskey standard), B (Whiskey) and B, which was very similar to the H sample (Original formula Whiskey). Even though the H sample (Original formula Whiskey) predicted as Whiskey Standard and Whiskey, the customer did not have an issue with this. The customer did not provide us a reason why the predictions were not an issue for the H sample.

Table III. Unknown Identifications using the C320

Sample Unknown	C320 Identification
50/50 Mix Whiskey & Gin	Unidentifiable sample
Original formula Whiskey	Whiskey Standard
50/50 Mix Whiskey & Gin	Unidentifiable sample
Original formula Whiskey	Whiskey
50/50 Mix Whiskey & Gin	Unidentifiable sample
Original formula Whiskey	Whiskey

4. Conclusion

The C320 was able to discriminate the distilled spirits into 5 distinct groups: Group 1 Rum and Vodka, Group 2 Whisky, Group 3 Gin, Group 4 Whisky Standard and Group 5 Gin Standard. The customer did not expect us to easily separate the two classes in Group 1 (Rum and Vodka). However, Rum and Vodka are of different colors, therefore a two-step process, using the C320 initially followed by a visual inspection, identification of all of the samples is possible. Once trained the C320 was successfully used to classify three test samples of 50/50 Mix Whiskey & Gin provided by the customer.

Figure 1. PCA plot of distilled spirits 40 proof at 75F

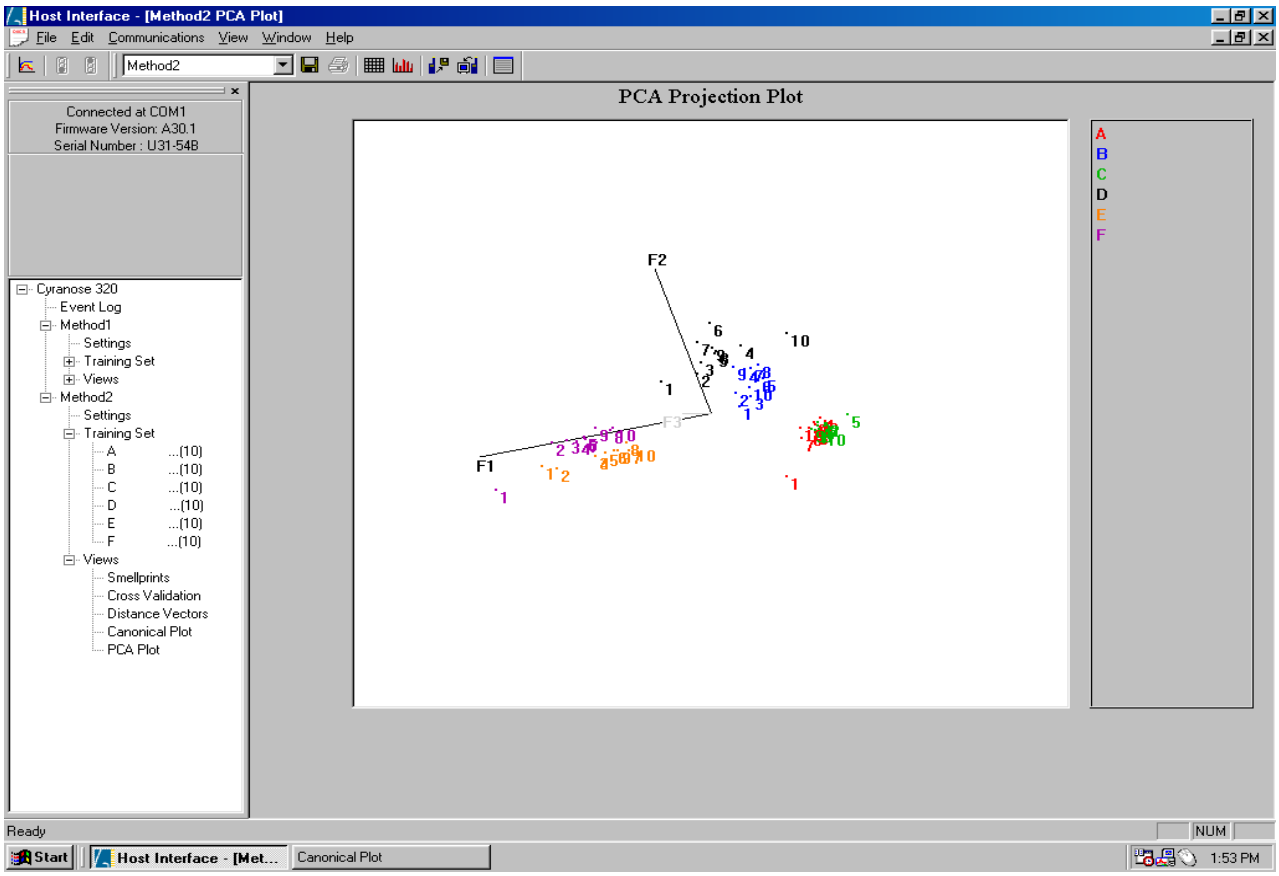

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Figure 2. Canonical plot of distilled spirits 40 proof at 75F

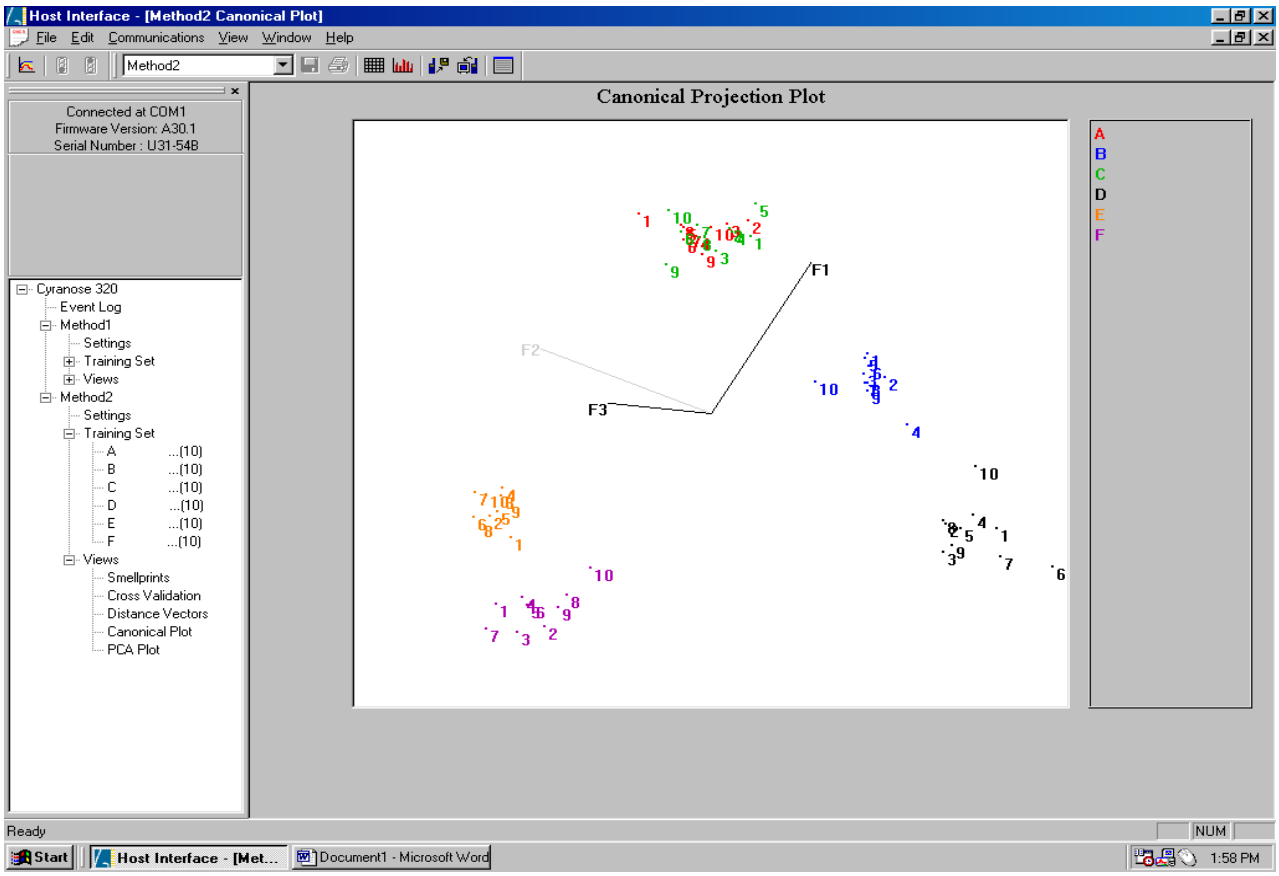

Figure 3. Cross Validation of distilled spirits 40 proof at 75F

Identified As

Trained As	A	B	C	D	E	F
A	7	0	3	0	0	0
B	0	10	0	0	0	0
C	4	0	6	0	0	0
D	0	0	0	10	0	0
E	0	0	0	0	10	0
F	0	0	0	0	0	10

Correct : 88.333 %
Incorrect : 11.667 %

Interclass M-Distances

	A	B	C	D	E	F
A		9.808	1.215	19.633	16.990	20.316
B			9.468	11.388	15.665	16.646
C				19.086	17.357	20.395
D					21.079	17.786
E						7.093
F						

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