**Application Note 19**
**Incoming Raw Material Inspection of Good Gasoline vs. Bad gasoline**

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## 1. Introduction

Chem-Trend, Inc. provided three gasoline samples, one good sample and two bad samples, for analysis. As raw materials shipped in, some gasoline has bad smell with it that is not acceptable by Chem-Trend, the company that is providing high quality products to its customers. Chem-Trend is seeking an objective means to do incoming raw material inspection. As learned from supplier, the bad gasoline may contain some aromatic sulfur compounds at ppm level. With Cyrano Sciences sensor technology, identification can be simplified by using the aroma signature of the headspace of the gasoline as an objective descriptor. To show the capability of this technology and Cyranose 320 for this application, a method was developed to analyze these gasoline samples.

## 2. Experimental

Sample preparation:
Experiment 1: Gasoline samples were shipped to us in 3 aluminum cans provided by Chem-Trend. The 1 ml samples were placed in 20 ml vials. Ten replicates were prepared for each sample. All samples were kept in sealed vials in a lab environment with ambient conditions.
Experiment 2: Three gasoline samples were used as they were in the aluminum cans that were kept in a lab environment with ambient conditions.

Testing Conditions:
Experiment 1: The Cyranose 320 (U111-23A) with a 32-sensor array was used to test these samples. The instrument was on overnight before the test. The method settings are in Table 1. The training set was obtained by sampling the 30 sealed vials randomly.
Experiment 2: The Cyranose 320 (U135-44A) with a 32-sensor array was used. The instrument was warmed up 6 minutes before the test. The method settings are the same as they described in Table 1. The training set was obtained by sampling three cans randomly, 10 times from each can.

Data handling:
Data was recorded with the 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 $(R_{max}-R_{min})/R_{min}$. The 32 sensor responses were then mean-centered (or autoscaled) and normalized. . Canonical discriminant analysis (CDA), an algorithm for pattern recognition, with auto-scaling and 1-normalization was used for model-making and identifications.

## 3. Results

From experiment 1:
All three samples clustered into different regions in Canonical space (Figure 1), despite not controlling for laboratory air, which provided the baseline and carrier flow. The training process took about 30 minutes. Prediction was done on the sealed vials after the training set was built. Eighteen samples were tested. Only one M sample misidentified as a Good sample.

From experiment 2:
All three samples clustered into different regions in Canonical space (Figure 2). The cross-validation result is shown in Figure 3. Prediction was done on 4 unknowns that Chem-Trend sent to us. Unknown #1 was identified as good for 3 times. Unknown #2 was identified as F for 3 times. Unknown #3 was identified as M for two times and one time it was identified as good. Unknown #4 was identified as good 3 times. From interclass M-distances, we can see that M is very close to good and F is very different from good. This observation has been confirmed by the certificates associated with the materials that M may contain about 5 ppm aromatic sulfur compounds and F may contains the aromatic sulfur compounds in the level of 10 ppm to 100 ppm. This indicates that M is very close to good.

## 4. Conclusion

Analysis with a Cyranose 320 created distinct patterns that allowed samples of good gasoline and two bad gasoline samples (M and F) to be identified. Sample preparation for was simple and it took only 30 minutes to train the Cyranose 320. Four unknowns were predicted correctly with 100% accuracy. The training set lasted at least three days for correct predictions by eliminating the first sniff of each sample.

In order to improve the robustness of the training set, further work is recommended to fine tune the parameters in the method, especially in the environment of the inspection site (or in the real location that the instrument will be used).

Table 1 Method settings for Chem-Trend sample test

| Method name | gasoline | |
|---|---|---|
| | | |
| Class 1 | good | |
| Class 2 | F | |
| Class 3 | M | |
| Class 4 | M1Class4 | |
| Class 5 | M1Class5 | |
| Class 6 | M1Class6 | |
| | | |
| Baseline purge | 10s | medium |
| Sample draw | 6s | medium |
| Sample draw 2 | 0s | medium |
| Snout removal | 0s | |
| 1st sample gas purge | 0s | high |
| 1st air intake purge | 5s | high |
| 2nd sample gas purge | 30s | high |
| 2nd air intake purge | 0s | high |
| | | |
| Digital filtering | On | |
| Substrate heater | On | 42 |
| Training repeat count | 1 | |
| Identifying repeat count | 1 | |
| | | |
| Active sensors | FFFFFFFF | |
| | | |
| Algorithm | Canonical | |
| Preprocessing* | Mean-centering | |
| Normalization | Normalization 1 | |
| Identification Quality | | Always Choose |

* Mean-centering was used for unit U111-23A and Autoscaling was used for unit U135-44A.

Figure 1. Canonical plot of three gasoline samples (U111-23A)

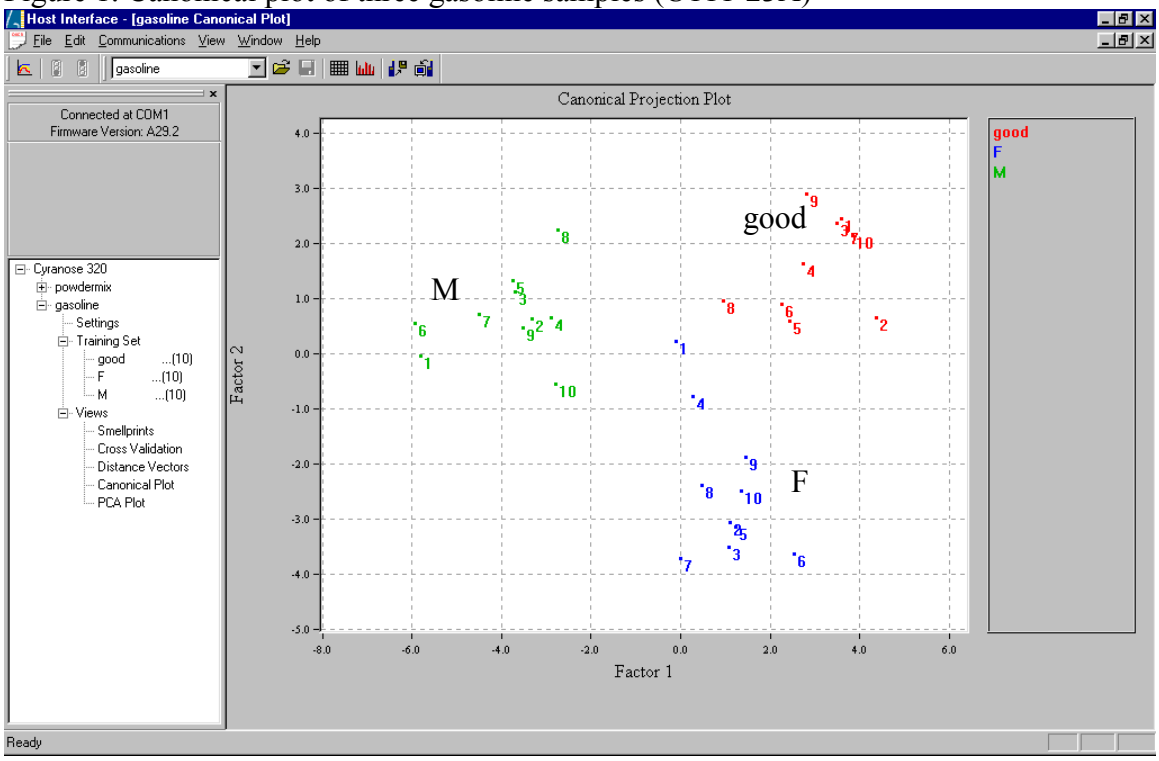
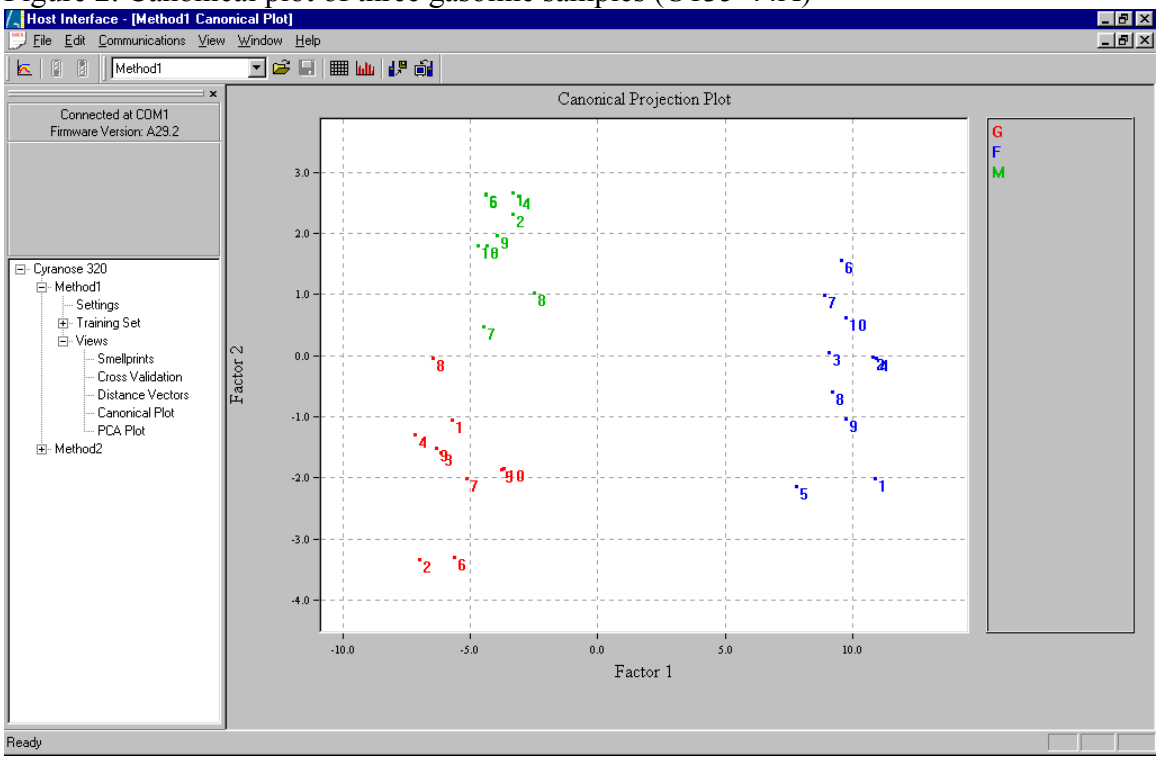



Figure 2. Canonical plot of three gasoline samples (U135-44A)

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