Application Note 20
Quality Control Screening of Plastic Pellets
Testing performed by: Cyrano Applications Group April 2001

1. Introduction

Off odors in plastic pellets represent a large problem for many different consumers of plastic pellets, from bottle manufacturers, consumers goods manufacturers to food packaging companies. The off odor may be due to residual hydrocarbon oils from the production steps or to specific compounds. Depending upon the operation an off odor may cause the process to be shut down, a costly experience for any plant, or if the plastic is nonetheless processed there may be an expensive product recall.

The Cyranose 320 (C320) could be used to detect the off odor at the incoming level before processing takes place or once the product is molded, ensuring your customers with higher grade product. This application note describes the use of the Cyranose 320 to identify PTFE and polypropylene plastic pellets with off odors.

2. Experimental

PTFE Samples
Sample Preparation:
Three samples of plastic pellet were tested: Control, Light odor and Bad odor. 10 samples of each type were placed in 40ml septum-lidded vials. Each sample contained 3 ±0.3 grams. All samples were stored in a lab environment at ambient conditions. The samples were heated to 100ºC for approximately an hour before testing was conducted at 100ºC.

Testing Conditions:
C320 with a 32-sensor array was used. Sensors 5, 6, 23 and 31 were deselected. All of the active sensors reached steady state response to the samples within the 15-second sample draw. The method settings are in Table I below. The training set was obtained by sampling vials randomly.

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.

Table I. Method Settings for PTFE pellets.

C320 Parameters	Time	Pump Speed
Baseline Purge	10 seconds	Low
Sample Draw	15 seconds	Low
Sample Draw 2	0	N/A
Snout removal	0	N/A
1st Sample Gas Purge	0	N/A
1st Air Intake Purge	10 seconds	High
2nd Sample Gas Purge	30 seconds	High
2nd Air Intake Purge	0	N/A
Digital Filtering ON		
Substrate Temperature 42°C	Sensors 5, 6, 23, 31 deselected	Algorithm used – Canonical, Autoscale, Normalization - 1

Polypropylene Samples:
Sample Preparation:
Three samples of plastic pellet were tested: Good, Borderline and Bad. 5 samples of each type were placed in 40ml septum-lidded vials. Each vial was approximately 25%filled with pellets. The samples were heated to 60ºC and then cooled to room temperature for testing.

Testing Conditions:
C320 with a 32-sensor array was used. All of the sensors reached steady state response to the samples within the 10-second sample draw. The method settings are in Table I below. The training set was obtained by sampling vials randomly.

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.

Table 2. Method Settings for Polypropylene pellets.

C320 Parameters	Time	Pump Speed
Baseline Purge	10 seconds	Low
Sample Draw	10 seconds	Low
Sample Draw 2	0	N/A
Snout removal	0	N/A
1st Sample Gas Purge	0	N/A
1st Air Intake Purge	10 seconds	High
2nd Sample Gas Purge	20 seconds	High
2nd Air Intake Purge	0	N/A
Digital Filtering ON		
Substrate Temperature 42°C	All sensors used.	Algorithm used – Canonical, Autoscale, No normalization

3. Results

PTFE pellets:
The C320 was readily able to discriminate between the Control, Light odor and Bad odor with the samples at an elevated temperature of 100°C. Figures 1, 2 and 3 illustrate the PCA, Canonical and Cross Validation plots for the samples at 100°C. Cross Validation is 100% and the interclass distance between the Control and Light odor was 8.0. The interclass distances between the Bad and the Control was 18.9 and the interclass distance between the Bad and Light off odor was 12.9. All of the interclass distances demonstrate clear discrimination between all samples.

Polypropylene pellets:
The C320 was readily able to discriminate between the Good, Borderline and Bad samples of polypropylene. Figures 4, 5 and 6 show the PCA, Canonical and Cross Validation plots for these samples. Cross Validation is 100% with interclass distances of 9.8 between the Good and Borderline samples and 19.3 between the Good and Bad samples. These distances represent a clear discrimination between these samples. Furthermore the unknown samples identified using this model were all correctly classified.

4. Conclusion

The C320 is clearly able to discriminate Good from Bad and Borderline (or Light Odor) plastic pellets. This experiment demonstrates the excellent potential of the C320 to identify unacceptable samples of PTFE or polypropylene pellets prior to processing or prior to use in consumer goods.

Figure 1. PCA of PTFE at 100°C

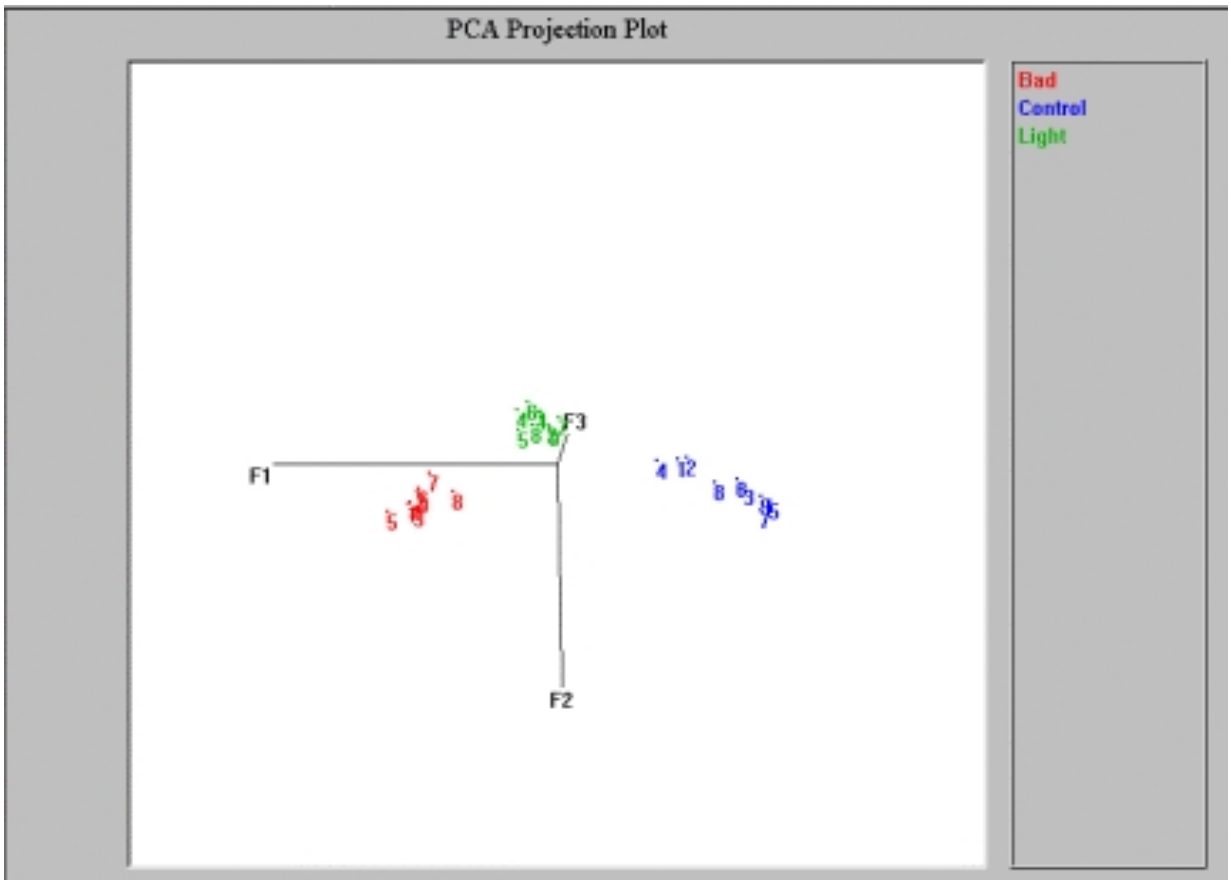

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Figure 2. Canonical plot of PTFE at 100°C

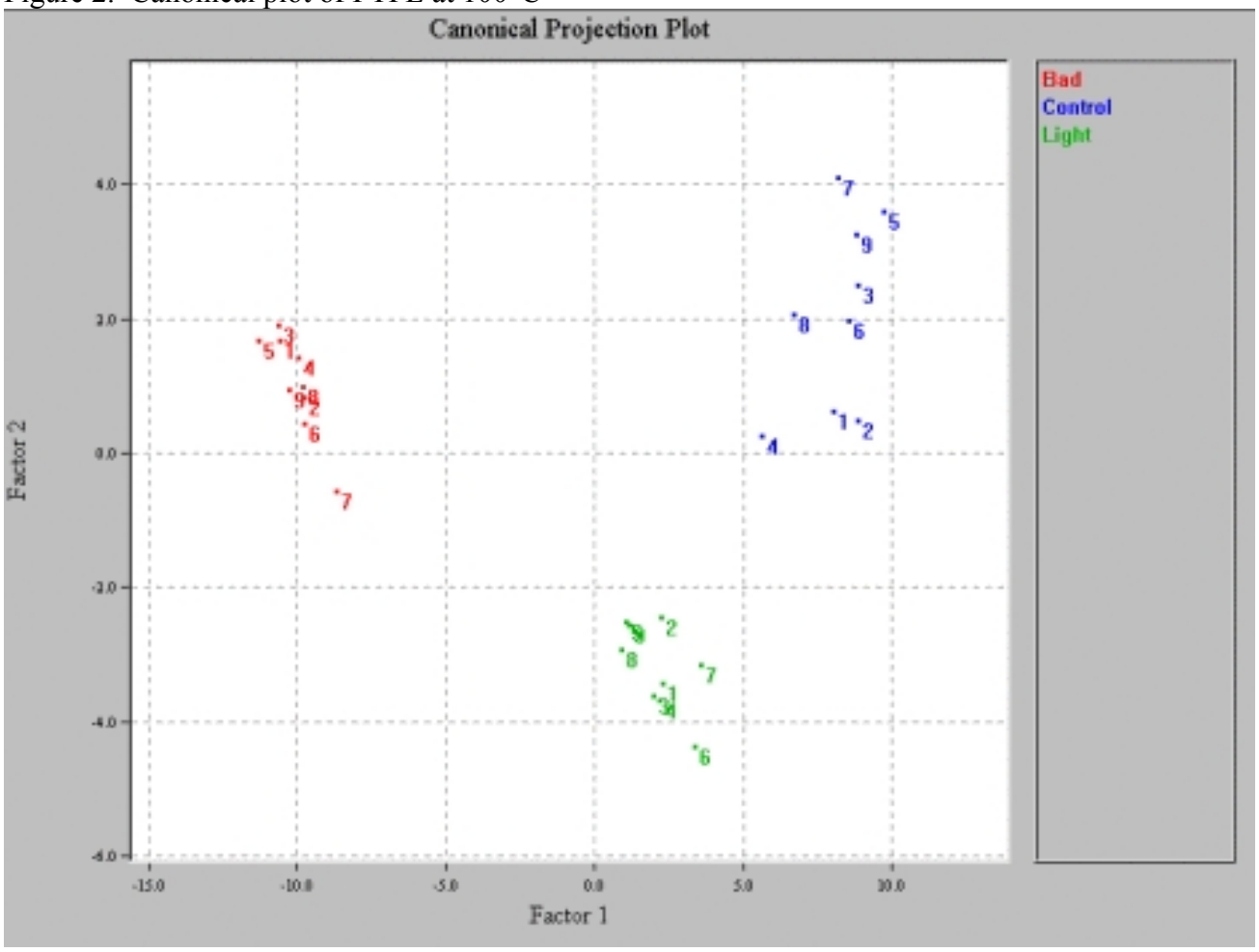

Figure 3. Cross Validation plot for PTFE at 100°C

Trained As

	Bad	Control	Light
Bad	9	0	0
Control	0	9	0
Light	0	0	9

Correct : 100.000 %
Incorrect : 0.000 %

Interclass M-Distances

	Bad	Control	Light
Bad		18.258	12.877
Control			8.038
Light			

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Figure 4. PCA of polypropylene pellets at room temperature.

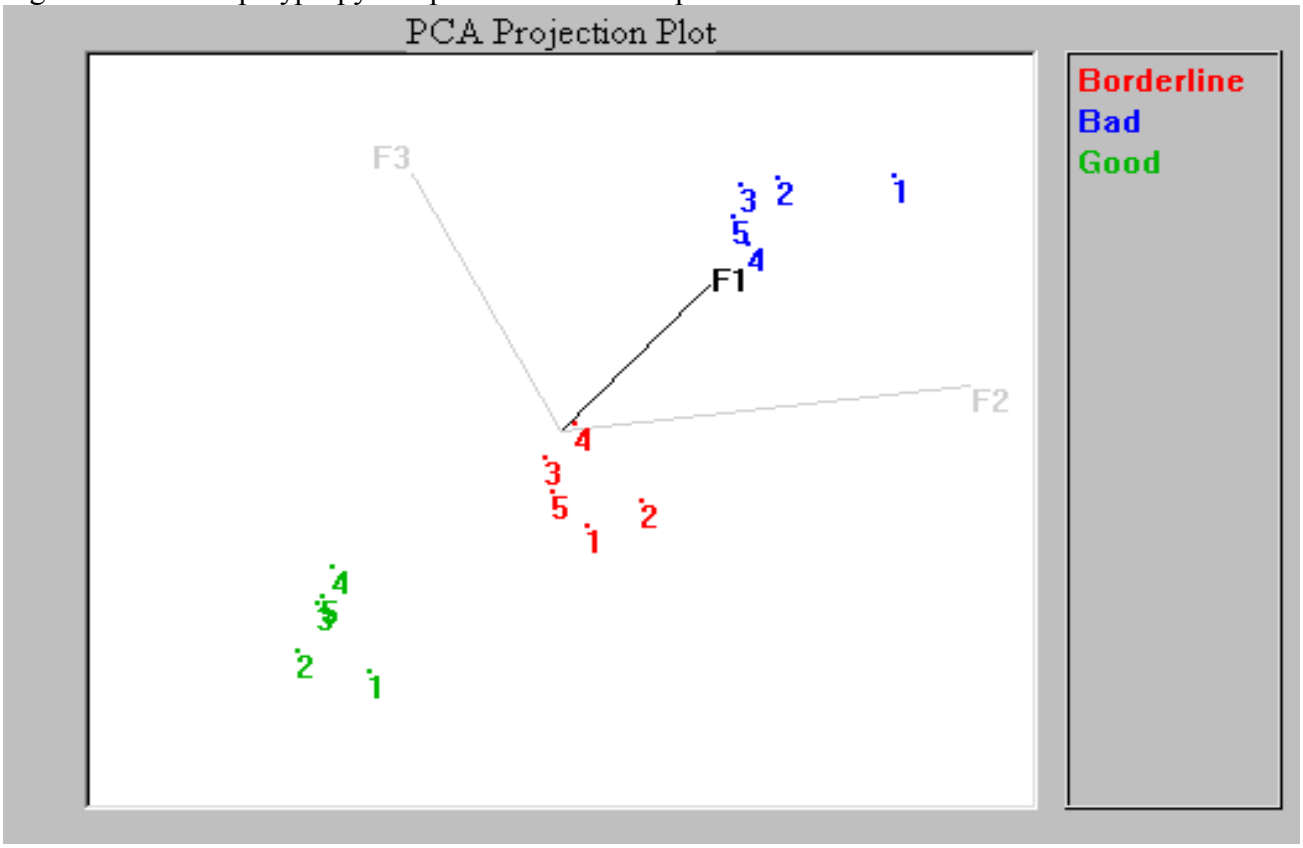

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Figure 5. Canonical plot of Polypropylene pellets at room temperature.

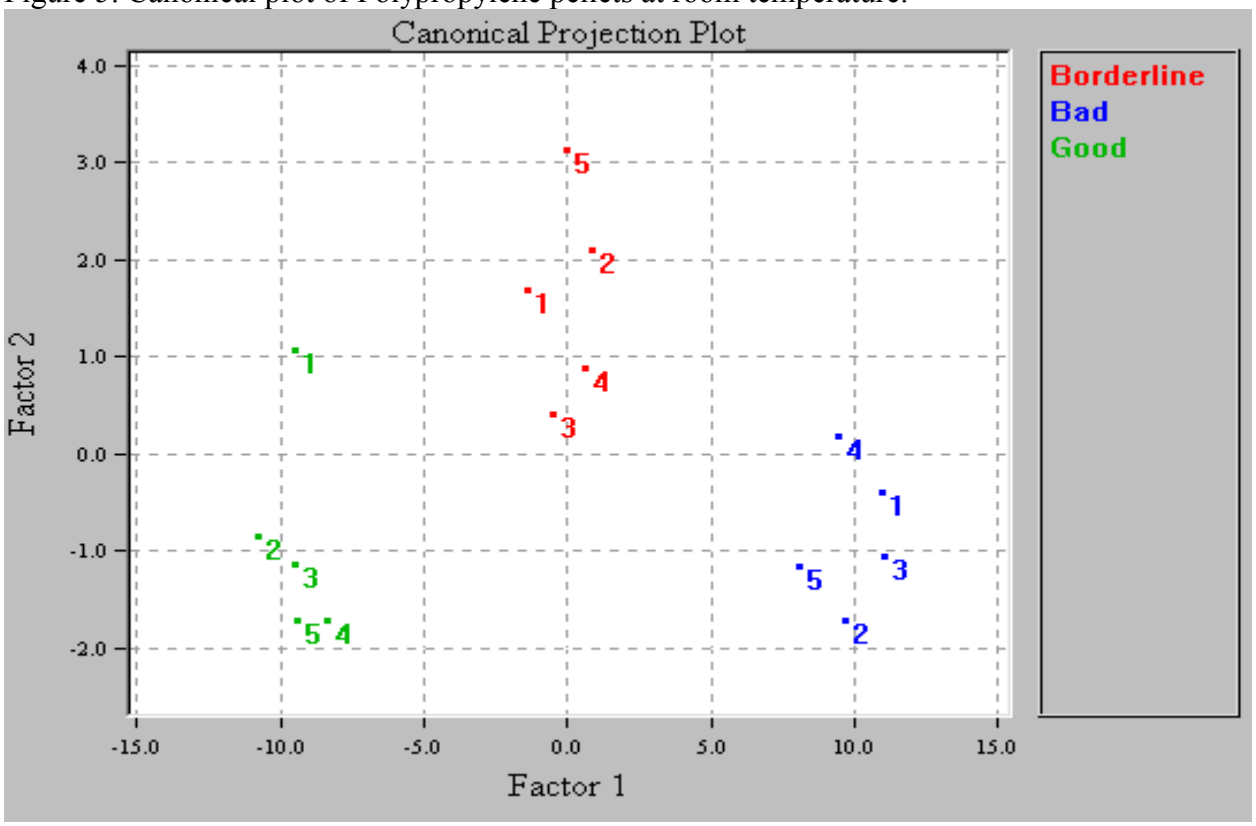

Figure 6. Cross Validation plot for polypropylene pellets at room temperature.

Identified As

Trained As	Borderline	Bad	Good
Borderline	5	0	0
Bad	0	5	0
Good	0	0	5

Correct : 100.000 %
Incorrect : 0.000 %

Interclass M-Distances

	Borderline	Bad	Good
Borderline		10.224	9.756
Bad			19.347
Good			

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