

Introduction:

The purpose of this study is to determine if flour premixes can be identified as within specification or not, using their NIT spectrum. This study is not meant to create a calibration or to prove the method, but to demonstrate that these products can be discriminated between the in or out of specification.

Description:

Fifty samples of flour premixes were provided for this study. Each sample was packed into a 5mm petrii dish and 10 scans were collected using the Series 3000 Food Analyser, between 720 and 1100nm. 12 samples from each of the in and out of specification batches were then combined into two library files called "Good" and "Bad" respectively.



Figure 1 below shows the standard absorbance spectra for all flour premixes.

Figure 1: Absorbance Spectra for all flour premixes.

The remaining samples were then analysed using the NTAS Discriminant Analysis software include in NTAS(NIR Technology Analysis Software). The Discriminant Analysis software calculates the Mahalanobis Distances between the unknown smaple spectrum and the library files. The library file with the lowest Mahalanobis Distance is selected as being the closest match.

Figure 2 below shows results of the Discriminant Analysis routine of an "In specification" or "Good" sample.

🗑 Discriminant Analysis 📃				
File Options Scanning Windows He				
Select the library files: GOOD.CSV BAD.CSV	3.16-			/
	2.97-			
	2.69-			
	2.70-			
	2.61-			
	2.52			
Add File Del File Results: 1.0.4754 GOOD.CSV 2.0.5275 BAD.CSV	2.34-			
4	2.25 2.230 720 730 740 750 760 770 78	0 790 800 810 820 830 840 850 860 870 8	80 890 900 910 920 930 940 950 960 970 980	990 1000 1020 1040 1060 1080
× Wavelength		Current <u>S</u> can: QD18s1	OVERATV	- Discriminate using
Y Wavelength	1100 📩			2nd Derivative
Glusters		<u>G</u> et Scan	Calibrate	Quit
Calculating distance to C	:\DOCUMENTS AND SE	TTINGS\PETER\DESKTOP\PREM	IIX\BAD.CSV group	2:32 PM 22/01/2009

Figure 2: Discriminant analysis results for a good product.



Figure 3 below shows Discriminant analysis of an "out of specification" or bad sample.

Figure 3: Discriminant Analysis of a "Bad" sample or "Out of Specification" product.

The table bellow shows the full list of samples and whether the sample was "Good" or "Bad" according to Discriminant Analysis routine.

Sample ID	Group	
QD10	Good	
QD12	Good	
QD16	Good	
QD17	Good	
QD23	Good	
QD30	Good	
QD31	Good	

QD13	Good		
QD18	Good		
QO20	Bad		
QO23	Bad		
Q024	Bad		
Q011	Bad		
Q012	Bad		
Q015	Bad		
QD32	Good		
QD33	Good		
Q003	Bad		
Q004	Bad		
Q007	Bad		
Q008	Bad		
QD24	Good		
QD25	Good		
QD26	Good		
QD27	Good		
Q016	Bad		
QO19	Bad		
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 Table 1: List of Validation Set Results.

Conclusion:

The spectra for both in and out of specification products cannot be visually identified from their spectra. However, the Discriminant Analysis software was able to accurately and reproducibly categorise the products into the correct groupings.

This analysis could be conducted on several of the range of analysers on offer by NIR Technology Systems that operates in the 720-1100nm spectral region. The Series 3000 Food Analyser was chosen because of the ease of sample loading.

It can therefore be concluded that the Series 3000 food analyser is capable of discriminating between the in and out of specification flour premixes supplied.