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EDITORIAL PAGE

Just what the world needs: another journal!

Actually, this is only a newsletter. The purpose of which is to share ideas about Near Infrared. This type of communication has been discussed at "500 Users' Club" meetings for several years now. Since I have been acting chairman of the "club" for two years, I felt some obligation to make a start.

If this issue appears to have no clear guidelines for articles, that was my intent. Any suggestion, comment, hint, yes even complaint is as welcome as a full research paper. A simple "I found that by \_\_\_\_\_ing my sample, the reproducibility was enhanced" could potentially help dozens of users. To this end, we would like to add a "Letters" section to our second newsletter. Since communication is the lifeblood of any science, we plan on having a User's Bulletin Board set up at the Pittsburgh Conference in March.

My hope is that Near Infrared can become as widespread and recognized as any of the other spectral ranges in spectroscopy. It, of course, will not be able to do everything for everyone. But, until the limits are defined, we can have a lot of fun in a rapidly growing field.

Sincerely,

Emil Ciurczak

"THE APPLICATION OF NEAR INFRARED REFLECTANCE SPECTROSCOPY IN TEXTILES"

By: Subhas Ghosh - Institute of Textile Technology

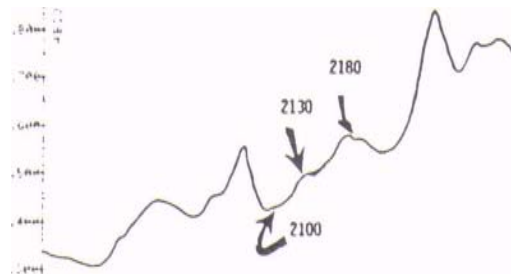
The use of near infrared spectroscopy, relatively new in the textile industry, has recognized its potential as a product and process control tool. Most textile testing specimens are in solid forms such as fiber, yarn, or fabrics. The InfraAnalyzer technology allows analysis of solid sample with very little preparation time. Most advantages of NIRA have been recognized in time savings over the conventional wet methods. We have recently investigated the use of near infrared spectroscopy to measure nylon fiber heat history.

Heat setting is one of the most critical parameters of synthetic fiber processing as it has significant effect on the molecular structure and the morphological response of yarns to further processing. This study deals with the carpet yarn heat history measurements using near infrared reflectance spectroscopy.

Present methods of estimating heat history using X-ray, DSC, IR, and other techniques are time-consuming and require technical expertise to perform the analysis, lowering the value of their application in a manufacturing situation. Therefore, NIRA was evaluated to measure yarn's heat history. In order to prepare a trial set for calibration of the instrument, a commercial Suesen heat setting range was used to prepare the learning temperatures ranging from 180° to 230° C.

The regression model for Nylon 6,6 yarns is reported in Table 1. A three filter model was selected using 2100, 2130, and 2180 nm filters. The correlation coefficient was 0.95 and regression F-ratio was 391.

Figure 1 illustrates a Near Infrared scan of Nylon 6,6. Three bands associated with the heat history measurements occurred at the wavelengths 2100 nm, 2130 nm, and 2180 nm. The band at 2130 nm was found to be the most critical wavelength for the heat setting temperature measurements. The analysis was performed by comparing the reported combination and overtone bands related to the observed peaks arising from the vibrations of the functional groups in nylon structure. The peak at 2130 is attributed to CH stretching vibration on a CO combination band. However, the peak at 2180 is associated with NH bend, a 2nd overtone arising from the the characteristic CO-NH grouping. It can also be related to CO stretching oscillation and amide third combination band in the nylon structure. No peak was observed at 2100 nm which may be attributed to the baseline correction for the 2130 peak due to the variation in sample preparation. The second derivative of the scan showing the rate of absorption of energy exhibited peaks at 2130 and 2180 nm as shown in Figure 2.



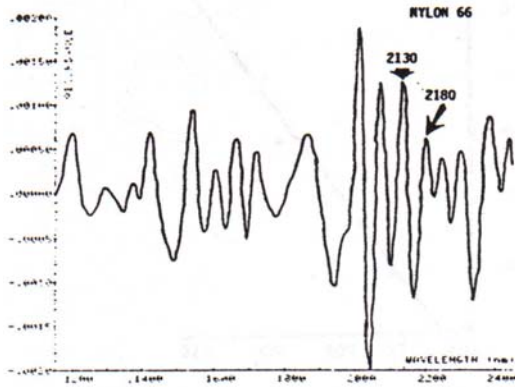


FIGURE 2.

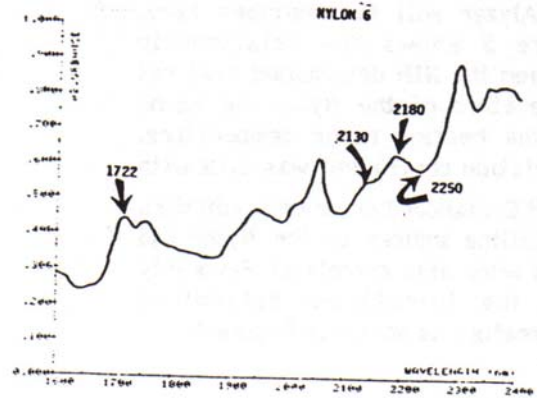


FIGURE 3.

The InfraAnalyzer was calibrated for Nylon 6 yarns also. A four filter regression model obtained for Nylon 6 yarns. The regression model obtained for Nylon 6 yarns is shown in Table II which included wavelengths 2130, 2180, 2250, and 1720 nm. A similar wavelength combination was found for Nylon 6,6 excluding the 1720 nm filter.

Figure 3 shows a NIR scan of Nylon 6 yarn which is similar to that of nylon 6,6. The bands at wavelengths 2130 and 2180 nm. have already been discussed. The peak at 1720 is related to CH stretching first overtone probably arising from CH<sub>2</sub>-CH<sub>2</sub> backbone in caprolactam. No peak was observed at 2250 nm, which may be attributed to the baseline correction. The second derivative of the scan shows distinct peaks at 1720, 2130, and 2180 nm. as illustrated in Figure 4.

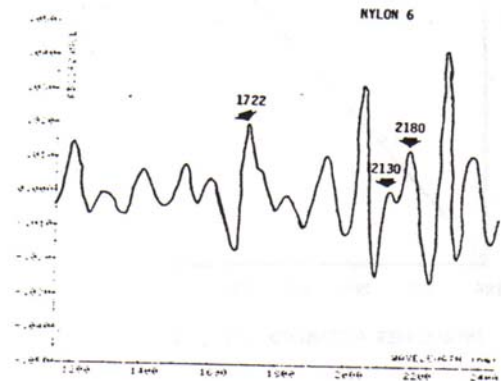


FIGURE 4.

When nylon yarns are annealed at temperatures well above the glass transition temperature, the crystalline fraction of the material increases because of the growth of large and more perfect crystals. This increase in structural order is associated with the change in configuration of the functional groups in the polymer chains from gauche to trans. The oscillations of these functional groups are related to the various wavelengths in the NIR regions as described earlier. Where the transformation of the functional groups occurs from gauche to trans due to the annealing changes.

Several researchers, including Starkweather, Noyniham, Sandeman, and Keller [1,2] have measured heat induced crystallinity changes in Nylon using infrared spectroscopy. They have found IR measurements correlated well with the density and X-ray measurements.

Some of the predictions of the InfraAnalyzer will be described here. Figure 5 shows the relationship between the NIR determined heat set temperature of the Nylon 6,6 yarns and the heating range temperature. Correlation coefficient was 0.98 with a 1.4° C standard error of prediction. Crystalline indices of the Nylon 6,6 yarns were also correlated favorably with the InfraAnalyzer determined temperature as shown in Figure 6.

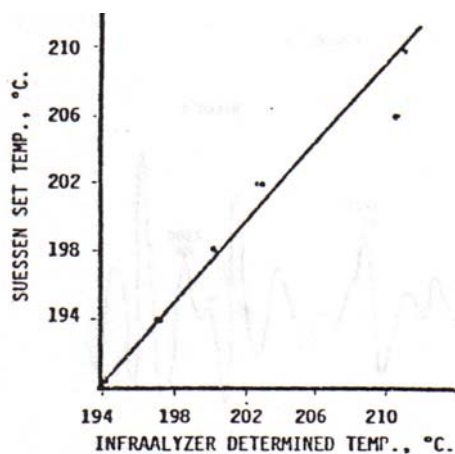


FIGURE 5.

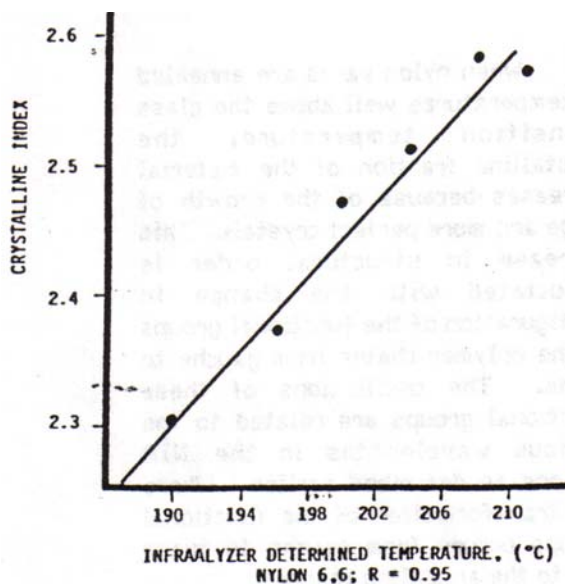


FIGURE 6.

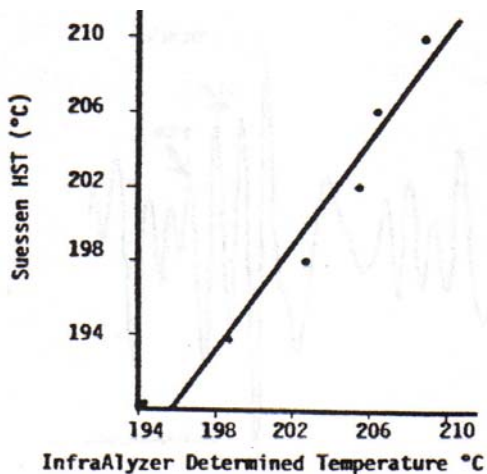


Figure 7.

Figure 7 illustrates the relationship between the InfraAnalyzer readings and actual heat set temperature for Nylon 6 yarns where the correlation coefficient was 0.99 and SEE was 1.50° C. Structural modifications of Nylon 6, also occurred due to heating, resulted in an increase in crystalline order as shown in Figure 3. The results presented here indicate that the InfraAnalyzer could be used to detect the heat history of Nylon yarns.

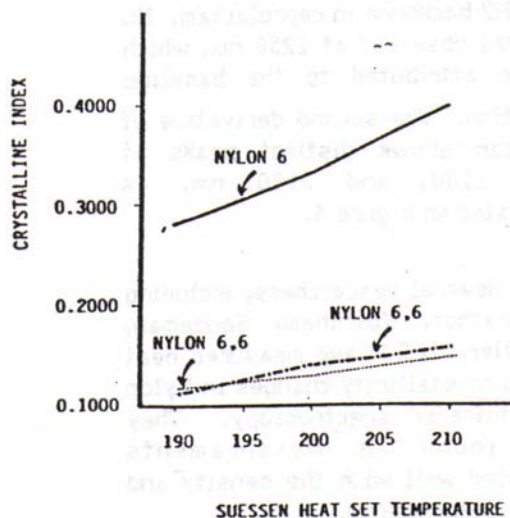


FIGURE 8.

Correlation of the NIRA data with X-ray diffraction measurements indicates that the NIR regression model detected the changes in the fiber structure and morphology due to the heat treatment.

ACKNOWLEDGEMENT

The author wishes to thank Dr. James E. Rodgers, Monsanto Fiber Intermediate Company for his valuable contribution in this work.

REFERENCES

1. Starkweather, Howard W., and Moynihan, Robert E., "Density, Infrared Absorption and Crystallinity in 66 and 610 Nylons", Journal of Polymer Science. Vol. XXII, pg 363-368
2. Sandeman, I. and Keller, A., "Crystallinity Studies of Polyamides by Infrared, Specific Volume and X-ray Methods", Journal of Polymer Science. Vol. XIX, pg. 401-435.

TABLE I.

NYLON 6.6 REGRESSION MODEL

WAVELENGTH (μ)	COEFFICIENTS
2.13	1618
2.18	-7672
2.10	-8744
"Y" INTERCEPT	423

TABLE II.

NYLON 6 REGRESSION MODEL

WAVELENGTH (μ)	COEFFICIENTS
2-25	-3969
0.99	
2.13	4643
161.2	
2.18	608
1.72	-1337
"Y" INTERCEPT	269

HOW ROBUST IS YOUR NIRA EQUATION

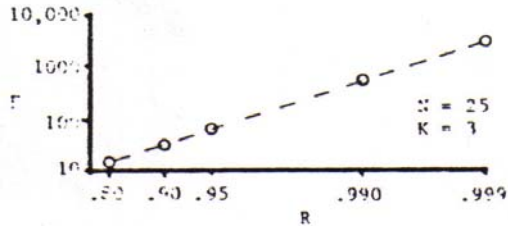
By: Don Burns - Technicon Science Center

Among the statistics which are printed during the calibration of an InfraAnalyzer, one (F) is a measure of so-called "robustness." Its properties are defined below:

$$F = \frac{R^2}{(1-R^2)} \frac{(N-K-1)}{K}$$

where R = correlation coeff  
 N = number of samples\*  
 k = # of wavelengths used

Clearly, F is influenced strongly by R; as the fit of the calibration line (or plane, or hyperplane, etc) to the observed points improves, R approaches unity and F achieves high values, (always exceeding 20)



The correlation Coefficient (R) is a function of two errors: the standard error of

estimate (SEE) and the standard deviation of the range (SD range).

$$R = \sqrt{1 - \frac{SEE^2 (N-K-1)}{(SD_{range})^2 (N-1)}}$$

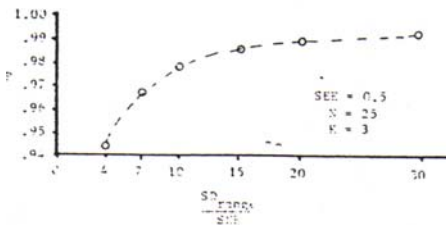
where SEE =

$$\sqrt{\frac{\sum(\text{InfraAnalyzer} - \text{Reference})^2}{(N-K-1)}}$$

The SD range should always be at least 10 x SEE, and the calibration range itself should exceed the range of interest (or, at the very least, equal it). R falls off rapidly as the ratio SD range drops below 10. SEE

\*Actually, number of scans in a data file. Beware of assuming that 10 triplicate scans is equivalent to 30 single scans; N=30 for both. F is calculated correctly only for the N single scan case.

F falls off less rapidly with a decrease in N.



## CONCLUSIONS

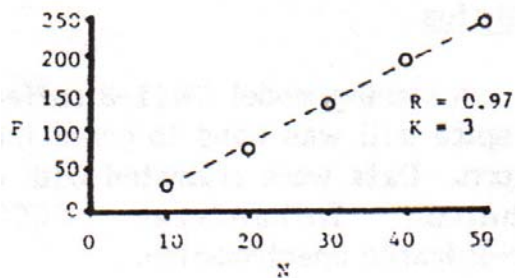
1. Have enough samples: 25-30 for one constituent; another 10 for each additional constituent.

2. Be sure they span the analytical range of interest.

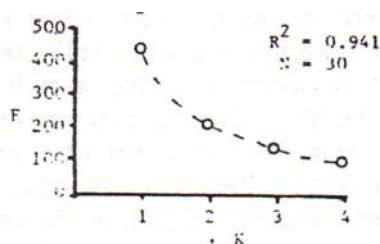
3. Use a reference method which will give a SEE not more than 1/10 the SD range.

4. If  $F < 20$ , the equation should not be used for determinations of unknown samples. In this case, reduce SEE (Which improves R).

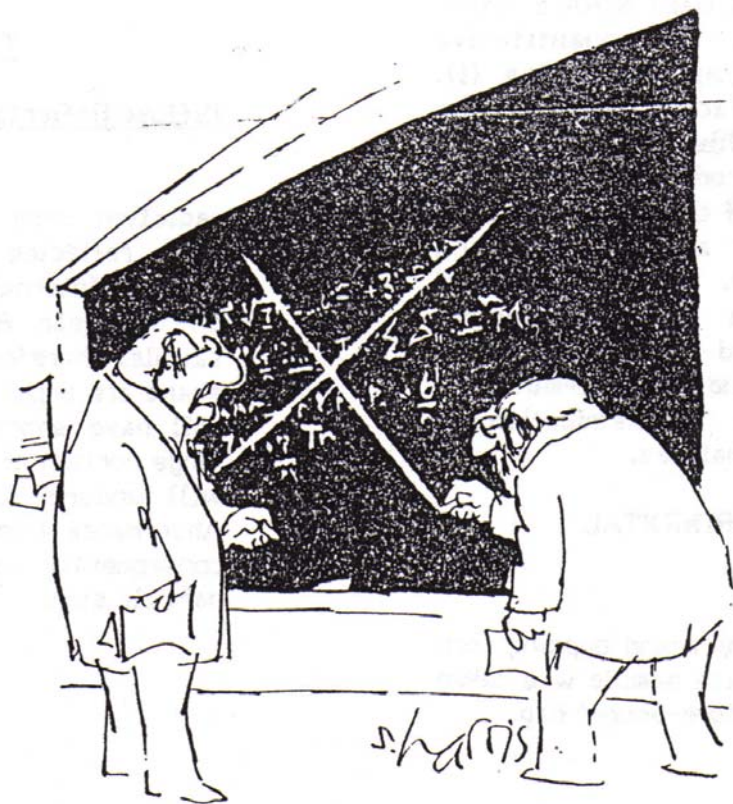
All of these statistics are available in the computer printout which accompanies the creation of a calibration equation. F-values can become enormous, and values in the range 100 to 50,000 aren't uncommon.



For a given level of correlation (e.g. constant R), F improves as the number of wavelengths required diminishes.



However, as an important wavelength is eliminated to reduce K, then R will suffer (decrease) and F will decrease even faster.



"THAT'S IT? THAT'S PEER REVIEW?"

# APPLICATION OF PRINCIPAL COMPONENT ANALYSIS TO NEAR INFRARED DIFFUSE REFLECTANCE PARTICLE SIZE DEPENDENCE

Michael D. DeGrandpre and David E. Honigs, Department of Chemistry, University of Washington, Seattle, Washington 98195

NIRA spectral variations from different particle size distributions were investigated. Popcorn was ground from 5-180 seconds and NIRA spectra were recorded. The analysis included three replicates of each sample. Principal component analysis was used to evaluate the data set. Results indicated significant replicate irreproducibility which could be minimized by increasing the number of replicates. In addition, it appears that an optimal grinding time can be predicted using the principal component model with a least squares regression.

## INTRODUCTION

Near-Infrared Reflectance Analysis (NIRA) depends on multivariate statistical techniques because of the complex spectra obtained. For multivariate analyses, subtle differences in sample spectra allow quantification of components of physical properties. Multiple linear regression has been successful in modeling these small spectral changes and has made NIRA a rather powerful tool for quantitative analysis of complex samples (1). Presently a factor limiting the sensitivity of this method is sample preparation reproducibility. Because of the nature of diffuse reflectance, spectra show a dependence on particle size (2). It is the intent of this study to examine spectral changes caused by particle size distributions and to determine the optimal particle size distribution for near-infrared analyses.

## EXPERIMENTAL

### Materials

Jolly Time brand popping corn was used and each sample was taken from the same store-bought bag.

### Apparatus

A Waring model CM11-8 coffee and spice mill was used to grind the popcorn. Data were collected with a Technicon InfraAnalyzer 500C Near-Infrared Spectrometer.

### Procedure

Approximately 60g of popcorn was loaded into the coffee grinder and grinding time was varied to obtain different particle size distributions. The grinding times ranged from 5-180 seconds (Table I). Near-Infrared spectra were collected immediately after all the samples were ground. The spectrometer scanned from 1000-2500 nm at 4 nm increments. PASCAL principal component analysis/multiple linear regression program (3) was used for the data analysis. Twenty-one wavelengths (every 50nm from 1500-2500 nm) were used in the analysis. It was assumed that all wavelengths would give the same amount of information or variance.

### THEORY

Diffuse Reflectance is the radiation from a surface that has been reflected within the sample matrix. Internal reflectance depends on the mean free path within the sample; therefore, particle size and shape are important. Small particles will have short wavelengths and a large portion of the incident photons will undergo diffuse reflectance. Absorbance ( $-\log[R]$ ;  $R$ =reflectance) consequently decreases for smaller particle size.

## Principal Component Analysis

Principal Component Analysis (PCA) was used to evaluate the spectra data matrix. Principle Components (PC's) explain the maximum amount of variance in a data set by using linear combinations o-f the intrinsic variables. The format shown below was used in the PCA algorithm (4):

In the matrix equation,  $X$ ,  $t$ , and  $p$  represent the data matrix and the principal component scores and loadings, respectively. Loadings are orthogonal "spectra" of the components which contribute to the total variance. Scores can be thought of as projection onto the principal component defined by the loadings. An iterative procedure was used to calculate the scores and loadings. A more rigorous outline of this procedure can be found in (5).

### RESULTS AND DISCUSSION

The sample spectra are shown in Figures 1-3 (see Table I for sample identification). As expected, increasing the grinding time increased reflectance indicating finer particle distributions. Figures 2 and 3 are included to show the irreproducibility among replicates and the differences of the samples with grinding times  $\geq 20$ s, respectively. Note that as grinding time increases the absorbance maxima to baseline difference decreases resulting in poorer sensitivity (signal-to-noise). It is evident that an optimum grinding time would maximize peak intensity while giving reproducible results. Selection of the optimum grinding as discussed later in this paper. First replicate reproducibility shall be examined.

In an ideal industrial process, any analyst effects would be eliminated by using an on-line NIRA spectrometer. When it is necessary

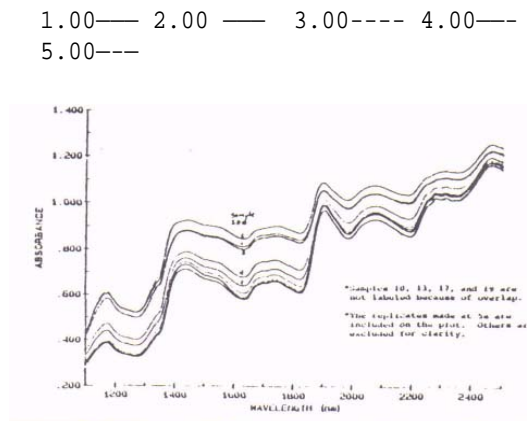


FIGURE 1: SAMPLE SPECTRA

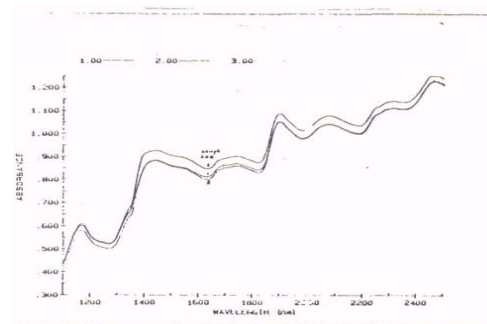


FIGURE 2: REPLICATE SAMPLE

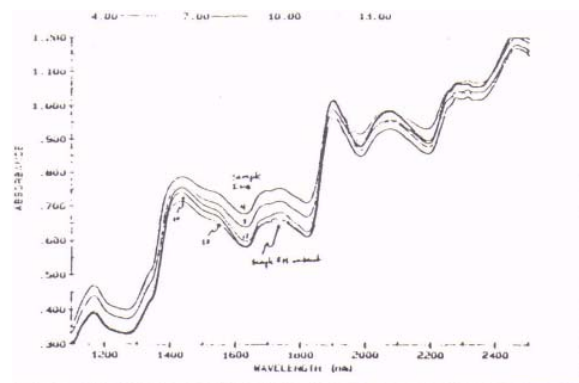


FIGURE 3: GRINDING TIME

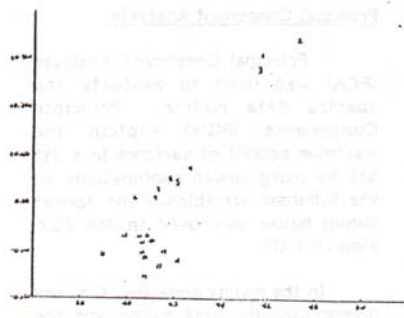
for the sample to be handled by and analyst, sample loading variations can be minimized by selecting specific guidelines for particular sample types. Nonetheless, identically handled replicate samples can have significant variations as seen in figure 2 (ave. std. dev. = 0.021 absorbance units). Depending on the precision desired, uncertainty can be reduced by simply increasing the number of replicates.

The data from samples 1-21 were analysed using principal component analysis. The first PC explained 99.88% of the variance within the accuracy of the analysis (+/- .005 absorbance units). The loading and scored are reported in Table II.

The first PC corresponds to the direction of variance from the different particle size distributions (grinding times) which was known to be the only variable in the data set. The remaining variance is a combination of noise and irreproducibility in the sample replicates. The loadings of the two principle components are plotted in Figure 4.

Note that the second PC does give some useful information. Separation of samples 4-9 from 10-21 is achieved whereas the first PC does not separate these sets. The second PC can not, therefore, be explained by completely random variations (noise).

As stated before, an optimal grinding time should consider both spectral intensity and reproducibility. The loadings for samples 10-21 ( $t \geq 60s$ ) indicate the ground popcorn has nearly reached a constant particle size. The minimum particle size will of course be dependent on the grinder or mill used. Grinding until there is essentially no more size reduction would be ideal from the reproducibility standpoint.



FIRST PRINCIPAL COMPONENT

FIGURE 4: PRINCIPAL COMPONENTS

TABLE I: SAMPLE GRINDING TIMES\*

Sample Number	Grinding Time(s)
1	5
2	
3	
4	20
5	
6	
7	30
8	
9	
10	60+
11	
12	
13	60+
14	
15	
16	120
17	
18	
19	180
20	
21	

\* Three replicates of each sample

+ Two samples - each ground 60 seconds

Grinding time could be increased as the blades or other mechanical parts of the grinder become worn. Regrettably, materials prepared as such will give the lowest peak intensity. To obtain an optimal grinding time one must consider samples 1-9.

Results of a least squares linear regression for samples 1-21 are given in Table III. Because there appears to be a linear relationship for samples 1-9, the correlation coefficient could be possibly be improved by excluding the samples where particle size is no longer changing (sample 10-21). The optimal grinding time would be selected within the range defined by the least squares line. An accurate line representing spectral variations versus grinding time could also be used to predict changes in the measured variables due to different particle size distributions.

Principal component analysis revealed two important aspects of particle size in NIRA: 1) the spectral intensity decreases linearly with increasing grinding time and 2) spectral variations are minimized by grinding until the particles reach a minimum size (this depends on the grinder or mill).

It should be noted that the results outlined in this report are strongly process dependent and each NIRA application would require its own characterization (i.e., a similar study could be extended to homogenization of liquids).

#### ACKNOWLEDGEMENTS

Sincere thanks to Professor Honig's research group for providing the instrumentation and software.

TABLE II FIRST AND SECOND PRINCIPAL COMPONENTS

SCORES		LOADINGS	
T1	T2	F1	F2
0.1744	0.2208	4.5723	0.3019
0.1700	0.2526	4.7192	0.3395
0.1575	0.3320	4.5579	0.2764
0.1563	0.3546	4.2703	0.0714
0.1693	0.2950	4.2139	0.0502
0.1710	0.2849	4.0270	0.0065
0.1629	0.3391	4.1301	0.0205
0.1755	0.2743	4.1783	0.0511
0.2407	-0.1514	4.1229	0.0068
0.2232	-0.0531	4.0532	-0.0810
0.2164	0.0051	4.0838	-0.0706
0.2319	-0.0784	4.0517	-0.0813
0.2318	-0.0795	3.9806	-0.0846
0.2227	-0.0199	4.1538	-0.1007
0.2175	0.0525	4.0750	-0.1154
0.2458	-0.0131	4.0757	-0.1142
0.2524	-0.1476	4.1330	-0.1369
0.2516	-0.1398	4.2043	-0.1212
0.2629	-0.2109	4.0738	-0.1535
0.2849	-0.2802	4.0970	-0.0825
0.2820	-0.2655	3.8973	-0.1119

1 = principal component #1

2 = principal component #2

TABLE III PRINCIPAL COMPONENTS LEAST SQUARES REGRESSION

$B_0 = -1.623 \times 10^3$	Root Mean Square = 42
$B_1 = 4.039 \times 10^2$	Correlation = 0.8936
$B_2 = 7.992 \times 10^2$	Degrees of Freedom = 18

#### LITERATURE CITED

- Honigs, David E. Anal. Instrum., 1985, 14, 1-54.
- Wetzel, David L. Anal. Chem., 1983, 55, 1165-1176.
- Perkins, Jonathan, unpublished notes, Laboratory of Chemistry, University of Washington.
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## STRANGE AND BIZARRE APPLICATIONS: SOMEONE, SOMEWHERE DID THEM

Edward Stark and Karen Luchter

### 1. How Many Eggs Are In Your Pasta?

For a spaghetti-eating Italian this is a real question which was solved by calibrating for a number of eggs. Sterols and fat were the measurement keys.

### 2. Do Your Plants Have A Digestive Disorder?

You know you are feeding your plants well - but even more important are they digesting what you give them and using your nutritious fertilizer and money to grow strong and healthy plant bodies? Bob Isaac sacrifices some leaves from his growing plants to get the answer with NIRA's help.

### 3. How Can I Measure What I Can't See? Or You Are Known By The Company You Keep.

Are you sure you can't see it? Yes there is no NIR absorbance for a carbon chlorine bond, nor for common table salt, sodium chlorine. But put a hydrogen on the same carbon with the chlorine and now the carbon hydrogen bond is effected by the chlorine through their shared carbon. The change in C-H bond strength changes the band absorption characteristics, particularly its position and voila! You can now indirectly

measure the chlorine through its environmental effect on the C-H bond. Similarly sodium chloride in water changes the H-O absorption band position of water and thus, the ion's effect is measurable.

### 4. Get Those Stones Out of My Chocolate!

Well, they are not really stones, only shells from the cocoa bean. It is hard on the eyes and fingers picking them out with tweezers but that is the current analytical technique until people started to experiment with near infrared correlations.

### 5. WANTED: Who Did the Original Cookie Diameter Work?

This application has come down through the lore and legend of NIRA but the infamous author and data has been lost to the obscurities of time and poor memories. As close as we can reconstruct it someone somewhere calibrated different flour mixtures against the resulting cookie diameters while keeping the stirring, water addition, baking temperature, and time constant. Please send any relevant information to the writers care of this publication.

## UPCOMING MEETING OF INTEREST

1. Pittsburgh Conference, Atlantic City, New Jersey March 10-11
2. 7th NIRA Symposium, Tarrytown, New York June 3-4
3. Rocky Mt. Analytical Soc., Denver, Colorado August 5-7
4. FACCS, St. Louis, Missouri September 28-October 3
5. Eastern Analytical Symposium, New York City, New York October 6-10

## RESEARCH DEFINITIONS

"IT HAS LONG BEEN KNOWN". . . . I haven't bothered to look up the original reference.

"WHILE IT HAS NOT BEEN POSSIBLE TO PROVIDE DEFINITE ANSWERS TO THESE QUESTIONS". . . . The experiments didn't work out, but I figured I could get a paper out of it.

"OF GREAT THEORETICAL AND PRACTICAL IMPORTANCE" .... Interesting to me.

"THREE OF THE SAMPLES WERE CHOSEN FOR DETAILED STUDY". . . .The results of the others didn't make sense and were ignored.

"ACCIDENTLY STAINED DURING MOUNTING". . . .Accidentally dropped on the floor.

"HANDLED WITH EXTREME CARE DURING THE EXPERIMENTS". . . .not dropped on the floor.

"TYPICAL RESULTS ARE SHOWN". . . .My best results are shown.

"PRESUMABLY AT LONGER TIMES". . . .I didn't take the time to find out.

"THESE RESULTS WILL BE REPORTED AT A LATER DATE". . . . Forget that one, baby!

"THE BEST VALUES WERE THOSE OF JONES". . . .He was a student of mine.

"IT IS BELIEVED THAT". . . . I think.

"IT IS GENERALLY BELIEVED THAT". . . . A couple of other guys think so too.

"IT MIGHT BE ARGUED THAT". . . . I have such a good answer for this objection that I want to make sure I get to use it.

"IT IS CLEAR THAT MUCH ADDITIONAL WORK WILL BE REQUIRED BEFORE A COMPLETE UNDERSTANDING". . . .Be damned if I understand it.

"CORRECT WITHIN AN ORDER OF MAGNITUDE" . . . .Wrong.

"IT IS HOPED THAT THIS WORK WILL STIMULATE FURTHER WORK IN THE FIELD". . . .This paper is not very good, but neither are any of the others on this miserable subject.

"THANKS ARE DUE TO JOE GLOTZ FOR ASSISTANCE WITH THE EXPERIMENT, AND TO JOHN DOE FOR VALUABLE ADVICE" Glotz did the work and John explained to me what it meant.

# FACSS XIII

## Monday AM/PM

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### **Near Infrared Analysis, arr. by Ed Stark, KES Associates**

Diffuse Reflectance in the Near and Mid Infrared Regions. **Peter R. Griffiths; University of California**

Interactance: A Spectroscopic Technique for Non-Invasive Analysis of Composition. **Karl Norris; Beltsville Agricultural Research Center**

Near Infrared Analysis Over an Optical Fiber. **David Honigs, Bruce Buchanan; University of Washington**

Foundations of Near Infrared Spectroscopy. **Wilbur Kaye; Beckman Instruments**

Fourier Transform Near-Infrared Spectroscopy: Techniques and Applications. D. **Kuehl, K. Krishnan; Bio-Rad, Digilab Division**

NIRA vs. FT/IR: A Study with Lignocellulose. **Donald A. Burns; Technicon Science Center. Tor P. Schultz; Mississippi State University**

Sensitivity and Linearity of an NIR Spectrophotometer in Comparison with FTIR. **Cynthia McDonald-Lewis; Pacific Scientific**

Moisture: Study of a Lively Near-Infrared Spectrum. **Gabor J. Kemeny, D.L. Wetzel; Kansas State University**

Applications of Near Infrared Spectroscopy: A Guide to the Future, **Kermit Whetsel; Tennessee Eastman**

NIRA Technology in the Mid Infrared. **Tomas Hirschfeld, Ed Stark, Stanley M. Angel; Lawrence Livermore National Laboratory**

Correlation Transform Spectroscopy in Fourier Space: Spectral Searching and Matching. **W.F. McClure; North Carolina State University**

NIR Qualitative Analysis by Spectral Matching. **Kathleen Ronan; Pacific Scientific**

Use of Derivative Nodes in Industrial Applications. **Lois Weyer; Hercules Inc.**

Criteria for Wavelength Selection Using an All-Possible Combinations Search Algorithm. **Jerome Workman, Howard Mark; Technicon Instrument Corp.**

## Tuesday PM

**Tomas Hirschfeld Memorial Symposium, arr. by D. Bruce Chase, E.I. DuPont de Nemours and Co.**

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Application of Some of Tomas's Ideas. **William G. Fateley; Kansas State University**

Designing Laboratory Robots for Optimal Functionality. **David Honigs; University of Washington**

The Legacy of Tomas Hirschfeld to Industrial Spectroscopy. **Jeanette G. Grasselli; Standard Oil Co.**

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