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THE USE OF NEAR INFRARED REFLECTANCE FOR EVALUATING COTTON FINENESS AND MATURITY

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ABSTRACT

The U.S. Department of Agriculture has proposed to develop a new high speed, high volume technique to assess cotton quality. This goal has led us to investigate the feasibility of near infrared reflectance spectroscopy as a technique for evaluating cotton fiber perimeter size and wall thickness, two of the physical characteristics used in the evaluation of cotton fineness and maturity.

In order to isolate the effects of perimeter size and wall thickness, nineteen cotton samples were selected on the basis of their having a nonsignificant correlation between these 2 measurements. The reflectance spectra from 1100 to 2500 nanometers was recorded at every other wavelength. The 700 independent variables were transformed by $\log(1/\text{reflectance})$. Due to the multicollinearity of the independent variables, the principle components were used in a multiple regression with data obtained from the reference method (arealometer) for the two dependent variables, perimeter size and wall thickness. The regression analysis of perimeter size and wall thickness on the principle components gave R^2 's of 0.229 and 0.943 respectively.

KEY WORDS: Cotton fineness, Cotton maturity, Near-infrared reflectance, Principal components.

1. INTRODUCTION

Cotton is a hollow fiber composed mainly of cellulose. The quality of the cotton fiber is determined by the various physical and chemical properties such as: perimeter size, wall thickness, length, percent moisture, percent protein and percent cellulose. Improved methods are needed to evaluate these properties that will save time and money, and provide greater reliability over existing techniques. The speed of the near-infrared reflectance spectroscopy (NIRS) method is comparable to that of the high volume instruments (HVI) already in existence. It is safe to use, is simple and inexpensive to operate, and is comparable to, and in some instances more accurate, than the existing techniques. Due to its versatility, we are evaluating NIR technology as a means to quantify cotton fineness and maturity.

We define cotton fineness as the perimeter of the cross-section of the fiber and cotton maturity as the fiber's wall thickness. Although they are correlated (the upper limit for wall thickness is a function of the perimeter ($\text{perimeter}/2\pi$)). ~~Accurate measurements of both characteristics are important for determining the~~ cotton's potential as fabric. Fiber perimeter size and wall thickness influence the ease with which fibers can be twisted during yarn formation. They influence the uniformity, lustre and stiffness of the fabric and the ability of the fabric to accept dye.

During the past 20 years near infrared reflectance technology has been used to quantify the chemical composition of a variety of agricultural products, such as the moisture content of grains, the oil content of soybeans, and the fat content of meat products (Panford, 1987). The NIR instrument operates like a "supermicroscope", in the region between the end of the visible and the beginning of the mid-infrared region (1100 - 2500 nm). It "sees" past the surface of the sample and penetrates into the molecules themselves (Fig. 1). The amount of incident light reflected from the sample relative to the amount of light striking it is measured at each wavelength in the NIR region. By an application of the Beer-Lambert law we are able to say that the concentration of a particular molecule is proportional to the amount of incident light reflected (Birth and Hecht, 1987).

Although NIR spectroscopy has been used successfully for a number of years to quantify the chemical constituents of agricultural products, it has not had widespread use in quantifying physical properties. This is particularly true in cotton fiber evaluation. Here, the lack of widespread use can be attributed to the complex morphology of the cotton fiber. To appreciate the complexity of the problem, some understanding of the growth process of cotton is essential. The cotton fiber is a tubular outgrowth of a single cell on the surface of a seed. Initially, the cell consists of a thin primary wall, composed mainly of cellulose. As the growing fiber approaches its final length, a secondary wall, also composed mainly of cellulose, starts to form on the inner surface of the primary wall. Eventually the boll splits open, the free moisture inside the boll evaporates, and the fibers dry. While drying, the fibers collapse from the circular cross-sectional shape to a variety of shapes which have been described as flat, bean, and horseshoe (Fig. 2) (Ramey, 1982).

The theory of how incident light is reflected and absorbed by hollow fibers has been poorly understood. But recently, Montalvo *et al.* (1987) have demonstrated that physical measurements of cotton fibers are linearly related to their NIR spectrum. A correlation ($p < 0.0021$) was found between the image analysis of cotton fibers and their NIR reflectance spectra. These relationships were retained ($p < 0.0317$) in cottons that had been purified by solvent extraction, but were nonexistent ($p > 0.1968$) in cottons that had the physical integrity of their fiber destroyed. Because of these encouraging results, a feasibility study was conducted to determine the potential of NIR reflectance as a technique for predicting cotton perimeter and wall thickness.

This paper reports the results of that study. Our objectives are to: (1) determine if NIR reflectance varies as a function of wall thickness and perimeter size; (2) to isolate identifiable effects; and (3) develop a statistical methodology and algorithm to predict wall thickness and perimeter size.

2. MATERIALS AND METHODS

One hundred one samples from the cotton producing areas of the U.S. were selected for the study. These samples were considered representative of the range of variability in perimeter size and wall thickness. All analyses were done in laboratories at standard conditions. This required the cotton samples to equilibrate for 24 hours at a temperature of 72°F and 40% relative humidity, before any analyses were done.

The cottons were analyzed for perimeter size and wall thickness using the standard method, the arealometer* (Hertel and Craven, 1951). The arealometer measures a cotton plug's resistance to air flow at two air pressures. This measure

*Mention of a commercial or proprietary product does not constitute endorsement by the USDA.

of resistance along with the length of the plug are used to calculate specific area (defined as the ratio of the external surface of the fibers to the volume of fibrous material) and immaturity ratio (defined as the ratio of the area of circle having the same perimeter as an average fiber to the actual cross-sectional area of the fiber). These values are used to calculate an indirect measurement of perimeter size and wall thickness. Two subsamples were taken from each of the 101 cottons, 2 to 3 additional sub-subsamples were then taken on each subsample. The means of the 2 subsample means were used as estimates for perimeter size and wall thickness.

The NIR measurements were done at the Southern Research Laboratory located in New Orleans, LA, on a computer-controlled, single-beam spectrophotometer (Research Composition Analyzer, Model 6350, Pacific Scientific, Silver Springs, MD). The computer program for data acquisition was based on sampling the spectra in the 1100 to 2500 nm range at even numbered wavelengths. Fifty spectral scans were taken for each sample and then averaged. The resulting 700 wavelength measurements per cotton were transformed by $\log(1/\text{reflectance})$. The $\log(1/\text{reflectance})$ is the standard transformation used on NIR reflectance data to establish a linear relationship between the optical data and concentration of the property of interest. This procedure is a direct result of the Beer/Lambert law which states, the concentration of an absorber is directly proportional to the ratio of the intensity of incident radiation divided by the intensity of the transmitted light radiation. Therefore a high $\log(1/\text{reflectance})$ value would indicate more radiation has been absorbed and less reflected by the cotton sample at that wavelength.

3. RESULTS

In order to determine if NIR reflectance varies as a function of perimeter size and wall thickness, four pairs of the original 101 cottons were selected based on the criteria: (1) perimeter sizes and wall thicknesses were both equal; (2) perimeter sizes were different and wall thicknesses were equal; (3) perimeter sizes were equal and wall thicknesses were different; and (4) perimeter sizes and wall thicknesses were both different. The perimeter size and wall thickness values for the selected cottons and the 95% confidence intervals of the means for the 101 samples are given in Table 1. The samples were selected to illustrate the effects that varying perimeter size and wall thickness have on the NIR spectra, the terms equal and different do not imply statistical significance. The graphs of the optical differences between the matched pairs of cottons were evaluated to determine if NIR reflectance varies as a function of perimeter size and wall thickness (Fig. 3).

Table 1. Perimeter size and wall thickness as measured by the Arealometer for the matched pairs of cottons.

COTTON	PERIMETER SIZE	WALL THICKNESS
ARS03	50.03	3.05
ARS11	45.46	2.26
ARS12	52.06	2.50
ARS18	42.54	2.82
ARS41	45.39	3.08
ARS47	43.35	3.13
ARS56	56.15	2.43

95% Confidence interval for perimeter size:
 mean \pm 4.216
 95% Confidence interval for wall thickness:
 mean \pm 0.384

of resistance along with the length of the plug are used to calculate specific area (defined as the ratio of the external surface of the fibers to the volume of fibrous material) and immaturity ratio (defined as the ratio of the area of circle having the same perimeter as an average fiber to the actual cross-sectional area of the fiber). These values are used to calculate an indirect measurement of perimeter size and wall thickness. Two subsamples were taken from each of the 101 cottons, 2 to 3 additional sub-subsamples were then taken on each subsample. The means of the 2 subsample means were used as estimates for perimeter size and wall thickness.

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95% Confidence interval for perimeter size:
 mean \pm 4.216

95% Confidence interval for wall thickness:
 mean \pm 0.384

In order to isolate the effects of perimeter size and wall thickness on the NIR spectrum, a subset of the original 101 cottons was selected. This subset consisted of 19 cottons that were representative of the range of variability (perimeter size mean=50.297+2.261 and wall thickness mean=2.699+0.417) and provided independent estimates of these measurements ($R^2=0.186$). This data set was used to evaluate the feasibility of using optical data as a means to develop a statistical model for predicting perimeter size and wall thickness.

Figure 4 displays the NIR reflectance spectra for the 19 cotton samples, $\log(1/\text{reflectance})$ vs. wavelength (nm). The graph shows some of the problems inherent in the optical data of cotton fibers: there are no clearly defined peaks, baseline variation is caused by particle size differences (larger particles change the direction of radiation less often), there are correlated measurements, and dispersion among the samples increases as a function of wavelength. A number of transformations have been proposed in the NIR literature to address the problems of baseline variation and increasing dispersion as a function of wavelength (Hruschka, 1987), but none have been applied to the optical data of hollow fibers. Therefore, 2 separate transformations were applied to the $\log(1/\text{reflectance})$ data: (1) a second derivative (series of finite differences); and (2) a multiplicative scatter correction (means were calculated at each wavelength and the 19 samples were then regressed against the mean) (Martens and Naes, 1987). Plots of the transformed data are displayed in Figures 5 and 6 respectively.

The correlated measurements and overlapping peaks pose a variable selection problem. In the absence of prior knowledge, wavelength selection can be approached by stepwise procedures, correlation plots, or all possible regressions. The R^2 's were calculated for perimeter size and wall thickness at each wavelength and the graph is displayed in Figure 7. Since the correlation plots offered little information as to which wavelengths measured perimeter size and wall thickness, we chose to avoid the variable selection problem by using principal components regression (PCR). PCR is a global calibration technique which uses all the independent variables to calculate a derived set of variables which preserves most of the information given by the correlations and covariances of the original set. These derived variables are then used in a regression analysis. If only some of the principal components are retained, the derived data set is less complex. In any case, the derived variables are uncorrelated.

The independent variable matrix X , was first centered for each wavelength and then replaced by its singular value decomposition (Mandel, 1982). For principle components regression this reduces to a (19×19) matrix U , the columns of which are the eigenvectors of the original XX' matrix and a (19×1) vector of unknown coefficients, calculated by the usual least squares solution $(U'U)^{-1}U'Y$, where Y is the (19×1) vector of dependent variables. In our case, only the first five principal components were retained as independent variables in a multiple regression to predict perimeter size and wall thickness.

4. RESULTS AND DISCUSSION

Figure 3 displays the NIR reflectance data as a function of changes in perimeter size and wall thickness. The graph clearly illustrates that the NIR spectrum varies as a function of these two properties. The difference spectrum for the first criteria where the values of both properties were equal is essentially zero, indicating their individual spectra are identical. When the perimeter size is varied while keeping wall thicknesses equal, the difference spectrum displays a baseline shift, indicating that less light is being reflected or more light is being scattered in the cotton with the larger perimeter size. In the third criteria, where wall thicknesses are varied and perimeter size remains equal, the difference spectrum

displays a baseline shift as well as a ramp effect, which could be an indication of particle size effect in the cotton with the larger wall thickness. When both properties are larger in one cotton than the other, we can conclude from the difference spectrum that the individual spectra are different. These results led us to conclude that the NIR spectrum varies as a function of perimeter and wall thickness.

In the data set containing the 19 cottons, we have isolated the effects of perimeter size and wall thickness. The second derivative transformation (Fig. 6) has eliminated the ramp effect, sharpened the peaks, and deconvoluted broad overlapping peaks into component peaks. However, there is still an indication of particle effect at the peaks. The transformation by multiplicative scatter correction (Fig. 7) eliminated the particle size effect and based on current NIR literature would lead us to believe this transformation would give us the best calibration model. A principal components regression was performed on data transformed by $\log(1/\text{reflectance})$, second derivative and multiplicative scatter correction. The $\log(1/\text{reflectance})$ gave the most promising results (Table 2). The

Table 2. Results of the principle component analysis for the 19 selected cottons.

PRIN. COMP.	% OF VARIANCE	CUMULATIVE %
1	97.800	97.800
2	1.706	99.506
3	0.306	99.812
4	0.132	99.944
5	0.047	99.991

first principal component accounted for 97.800% of the total variance. The regression analysis with the first 5 PC's gave an R^2 of 0.229 for perimeter size and an R^2 of 0.943 for wall thickness.

In light of our limited success, we decided to go back and reevaluate the arealometer data. A blind study was conducted using the 101 cottons, 2 samples were taken from each cotton and 2-3 determinations were taken on each subsample. We conducted a variance component analysis using a nested design structure. The relative variabilities are graphed in Figure 8. The large variability within the sample determinations for perimeter size indicate that its use as an independent variable in a PCR analysis is of limited value.

5. SUMMARY

We conclude that the NIR reflectance spectra contain information about cotton fiber perimeter size and wall thickness. The spectroscopy method is sensitive to small changes in fiber properties and therefore has the ability to independently predict perimeter size and wall thickness. Providing a sufficient number of determinations from the arealometer are made, PCR can be used to develop an algorithm to predict wall thickness. Due to the large variability in arealometer measurements within the sample determinations for perimeter size, its ability to be predicted through NIR analysis cannot be assessed.

6. REFERENCES

- G.S. Birth and H.G. Hecht (1987), "The Physics of Near-Infrared Reflectance," in *Near-Infrared Technology in the Agricultural and Food Industries*, eds. P. Williams and K. Norris, St. Paul, Minn.: American Association of Cereal Chemist, Inc., pp. 1-15.
- K.L. Hartel and C.J. Craven (1951), "Cotton Fineness and Immaturity as Measured by the Arealometer," *Textile Research Journal*, 21, 765-774.
- W.R. Hruschka (1987), "Data Analysis: Wavelength Selection Methods," in *Near-Infrared Technology in the Agricultural and Food Industries*, eds. P. Williams and K. Norris, St. Paul, Minn.: American Association of Cereal Chemist, Inc., pp. 35-56.
- I.T. Jolliffe (1986), *Principal Component Analysis*, New York: Springer Verlag.
- John Mandel (1982), "Use of the Singular Value Decomposition in Regression Analysis," in *The American Statistician*, vol 36, no. 1, pp. 15-24.
- H. Martens and T. Naes (1987), "Multivariate Calibration by Data Compression," in *Near-Infrared Technology in the Agricultural and Food Industries*, eds. P. Williams and K. Norris, St. Paul, Minn.: American Association of Cereal Chemist, Inc., pp. 57-88.
- J.G. Montalvo, Jr., D.P. Thibodeaux, S.E. Faught and S.M. Bucu (1987), "Prediction of Cotton Fiber Maturity by Near-Infrared Reflectance Analysis. Part I. Underlying Cause of Relationship", in *Proceedings of the Beltwide Cotton Production Research Conference*, pp. 155-165.
- J.G. Montalvo, Jr., S.E. Faught and S.M. Bucu (1989), "An Investigation of the Relationship Between Cotton Fineness and Light Scattering From Thin Webs as Measured by Near-Infrared Transmission Spectroscopy," *Applied Spectroscopy* (in press).
- J.A. Panford (1987), "Application of Near-Infrared Reflectance Spectroscopy in North America," in *Near-Infrared Technology in the Agricultural and Food Industries*, eds. P. Williams and K. Norris, St. Paul, Minn.: American Association of Cereal Chemist, Inc., pp. 201-212.
- H.B. Ramey, Jr. (1982), *The Meaning and Assessment of Cotton Fibre Fineness*, Manchester, United Kingdom: International Institute for Cotton.

Figure 1. Diffuse Refelctance. Incident light penetrates the surface of the sample and is reflected back. The incident light that is reflected back is recorded by detectors in the instrument. A ratio of the reflected/initial incident light at specific wavelengths provides information about the chemical and physical structure of the sample.

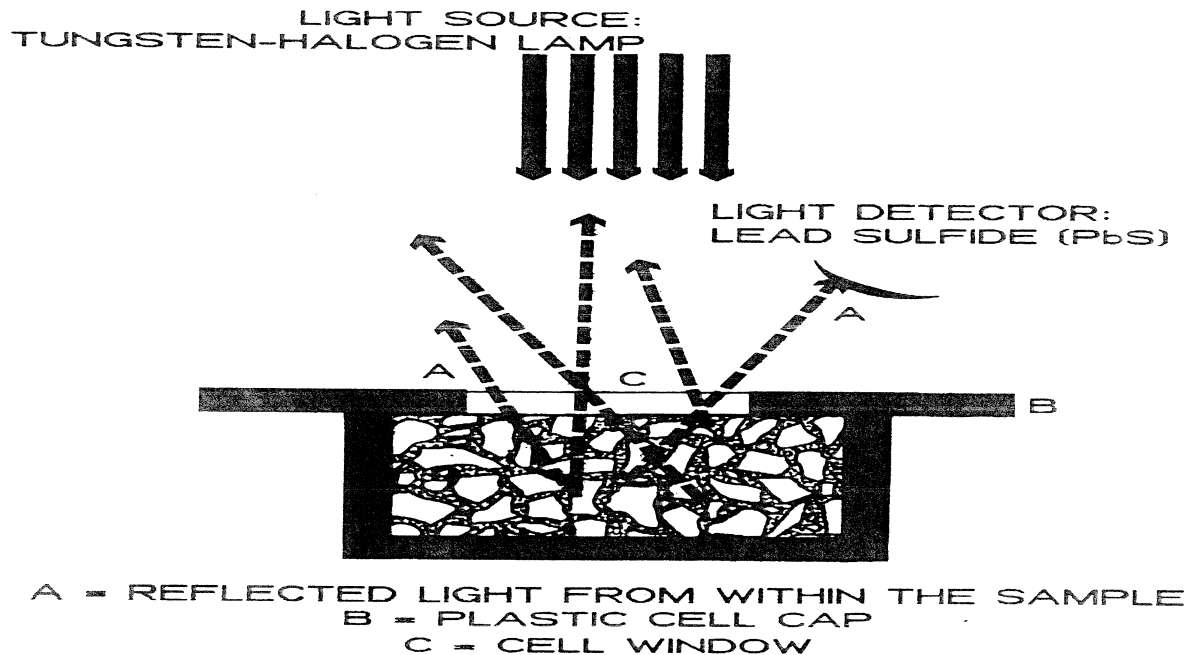


Figure 2. Cotton Fiber Cross Section. Initially the cotton wall is very thin, as it matures layers of cellulose are added to the wall. A few days prior to opening the cell wall ceases to grow. Once open, free moisture escapes and the cotton fibers collapse to form the various shapes.

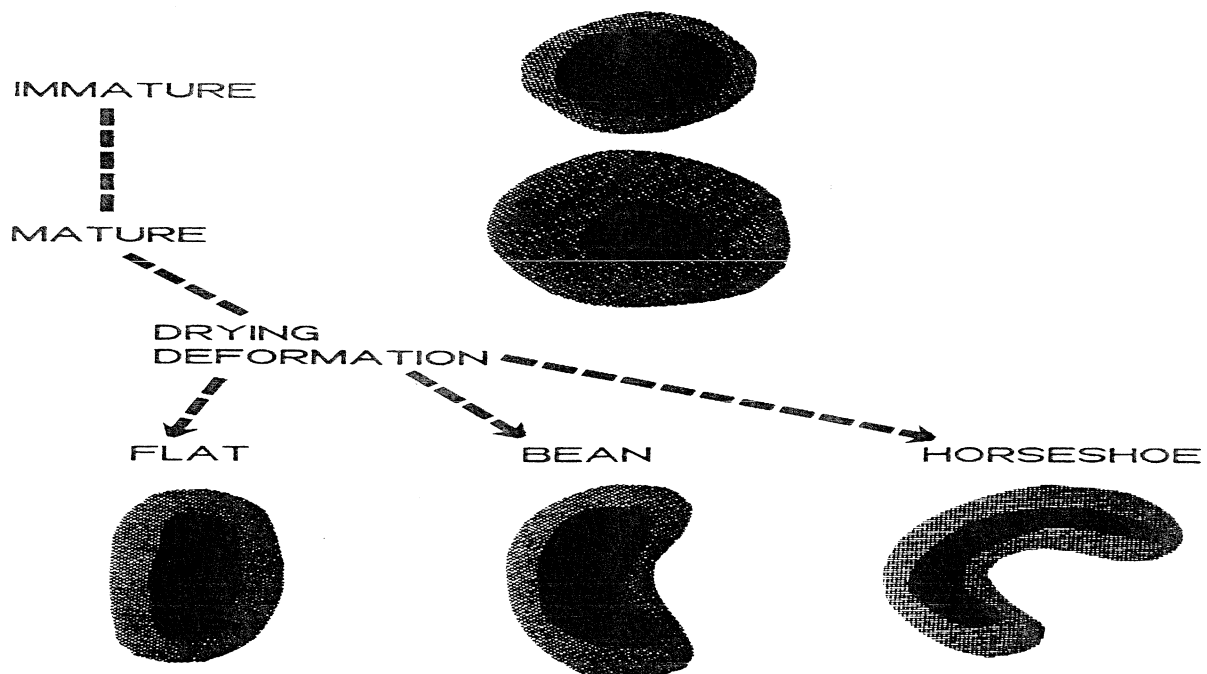


Figure 3. Wavelength (nm) vs. Log(1/reflectance). NIR diffuse reflectance spectra for the difference between pairs of cottons matched on four perimeter size (P)/wall thickness (T) criteria.

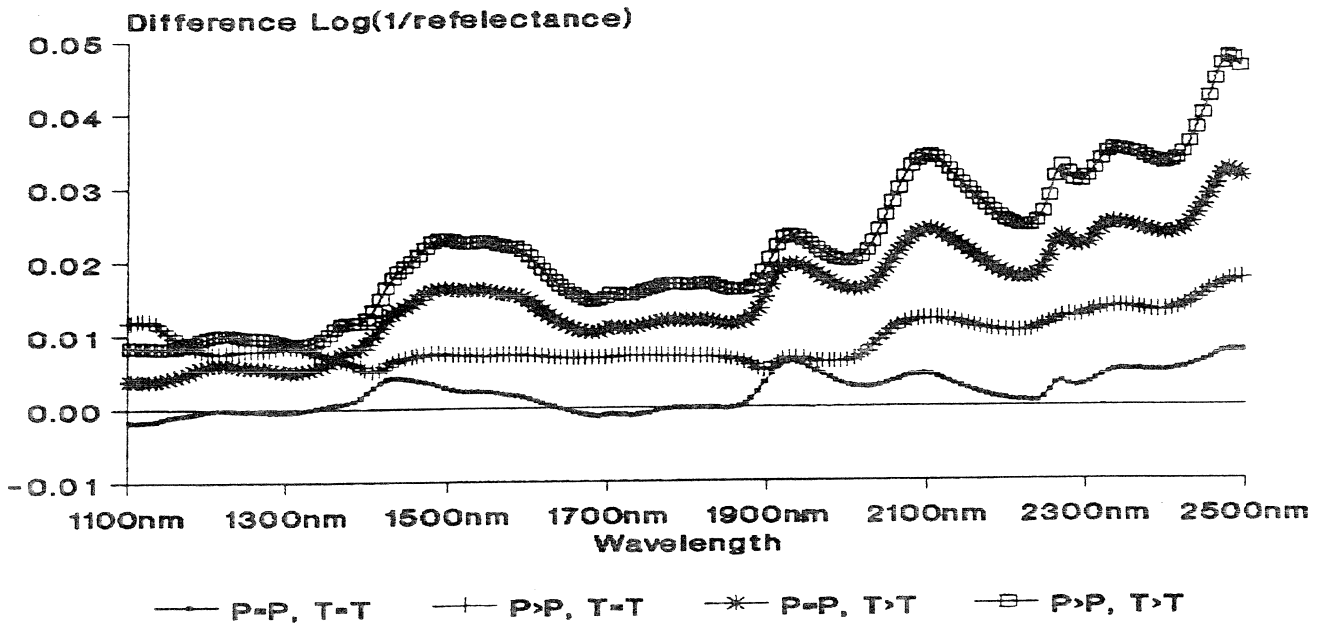


Figure 4. Wavelength (nm) vs. Log(1/reflectance). Diffuse reflectance spectra for the 19 selected cottons.

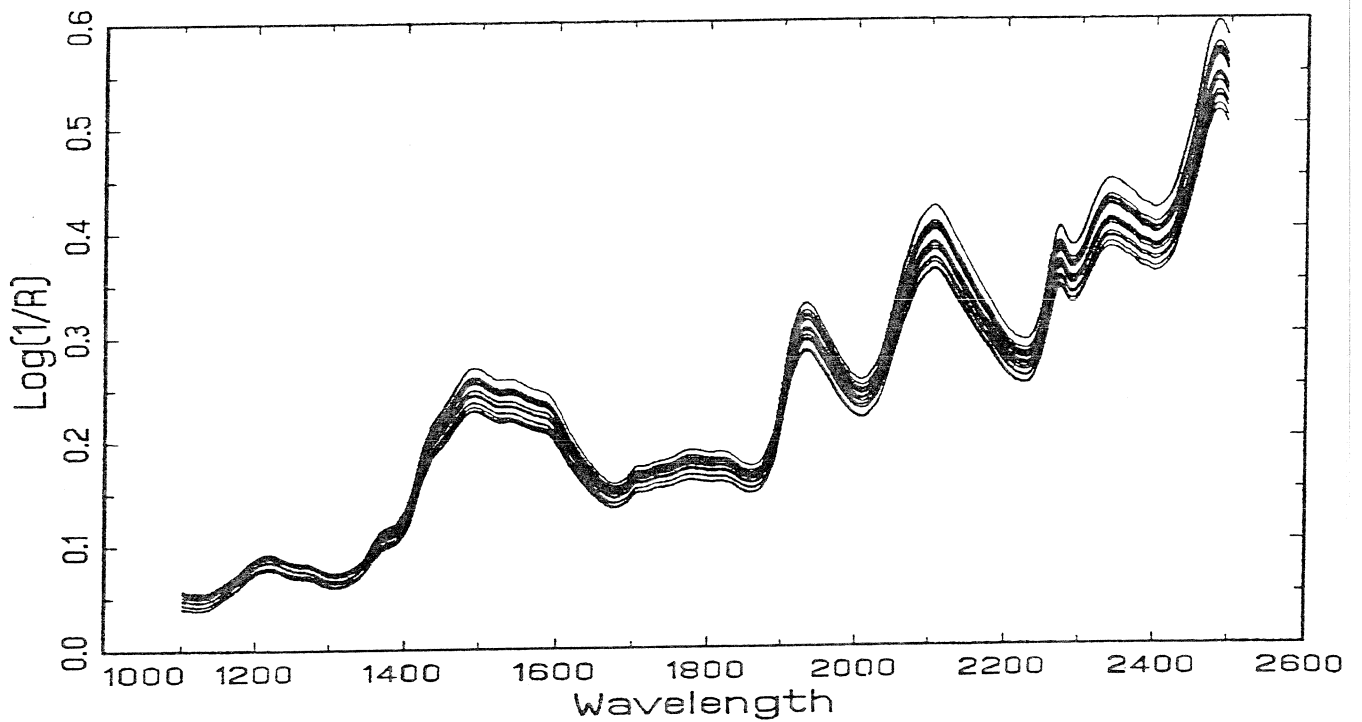


Figure 5. Wavelength (nm) vs. Second Derivative of the $\text{Log}(1/\text{reflectance})$. Diffuse reflectance spectra for the 19 selected cottons.

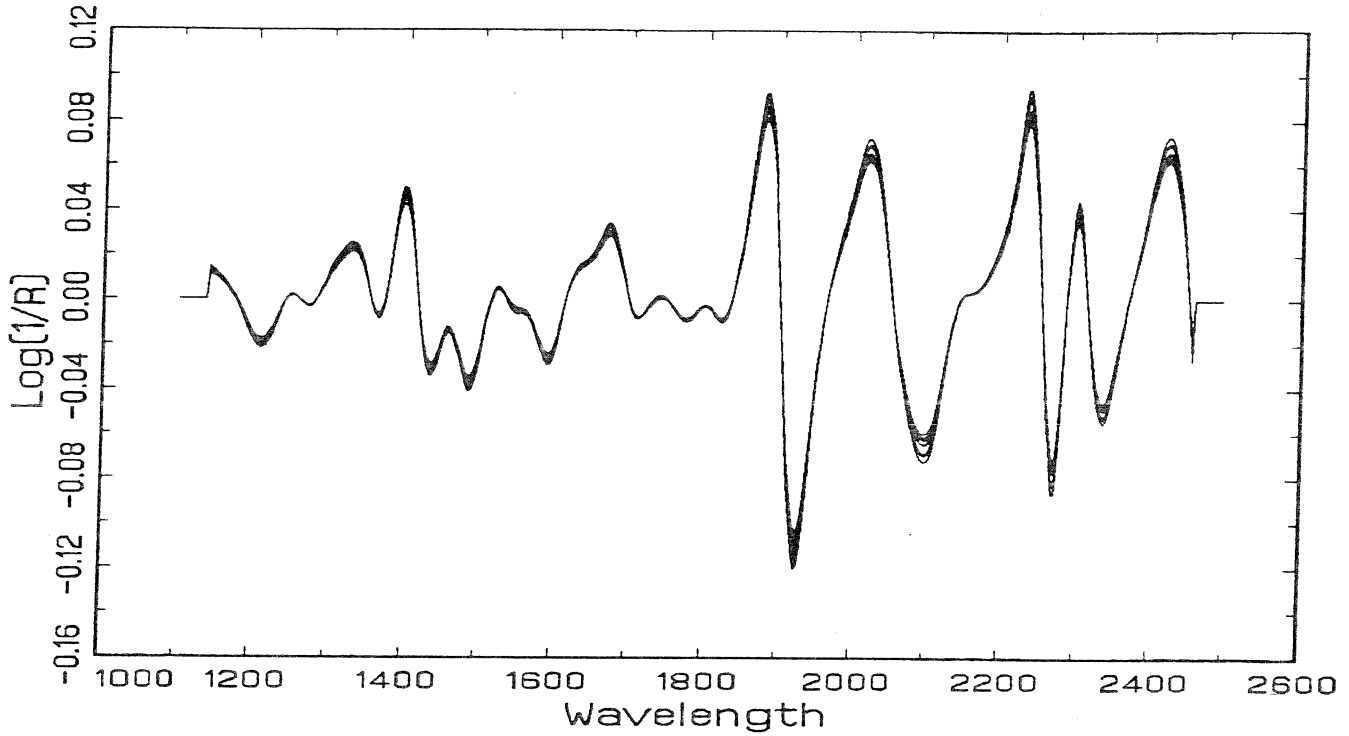


Figure 6. Wavelength (nm) vs. Multiplicative Scatter Correction of the $\text{Log}(1/\text{reflectance})$. Diffuse reflectance spectra for the 19 selected cottons.

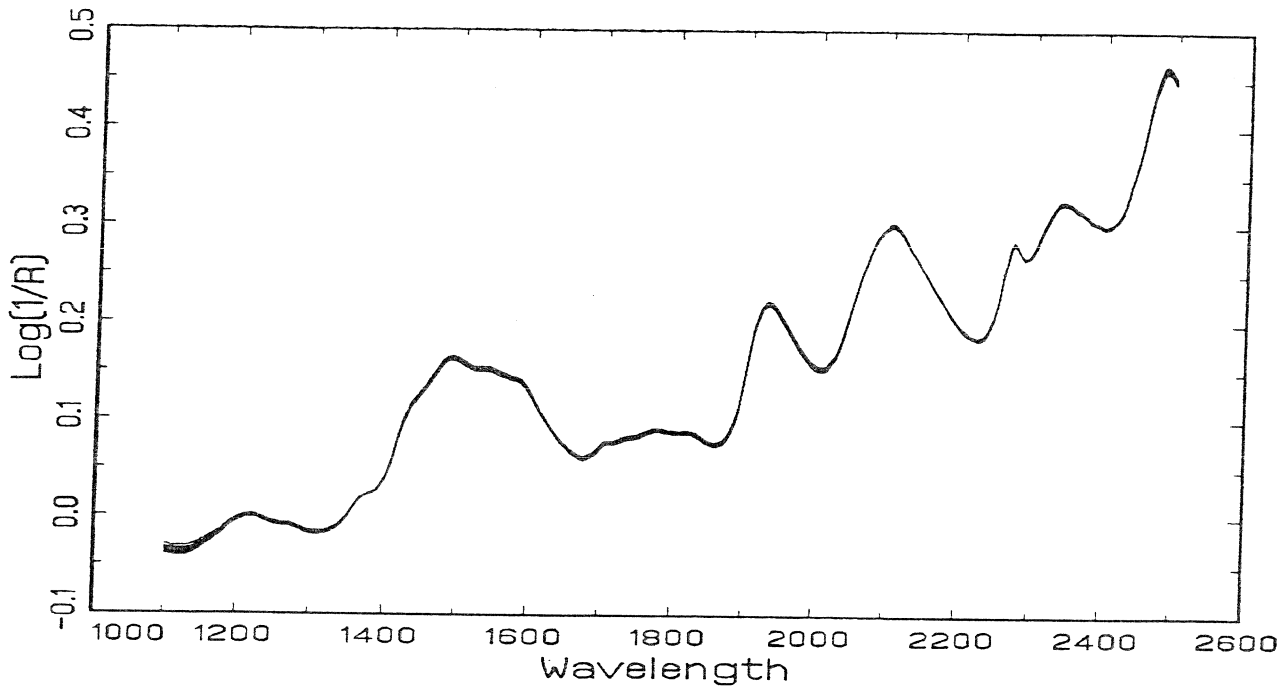


Figure 7. Wavelength (nm) vs. R^2 . Correlation plot for the 19 selected cottons. R^2 is calculated at 700 wavelengths for perimeter size and wall thickness.

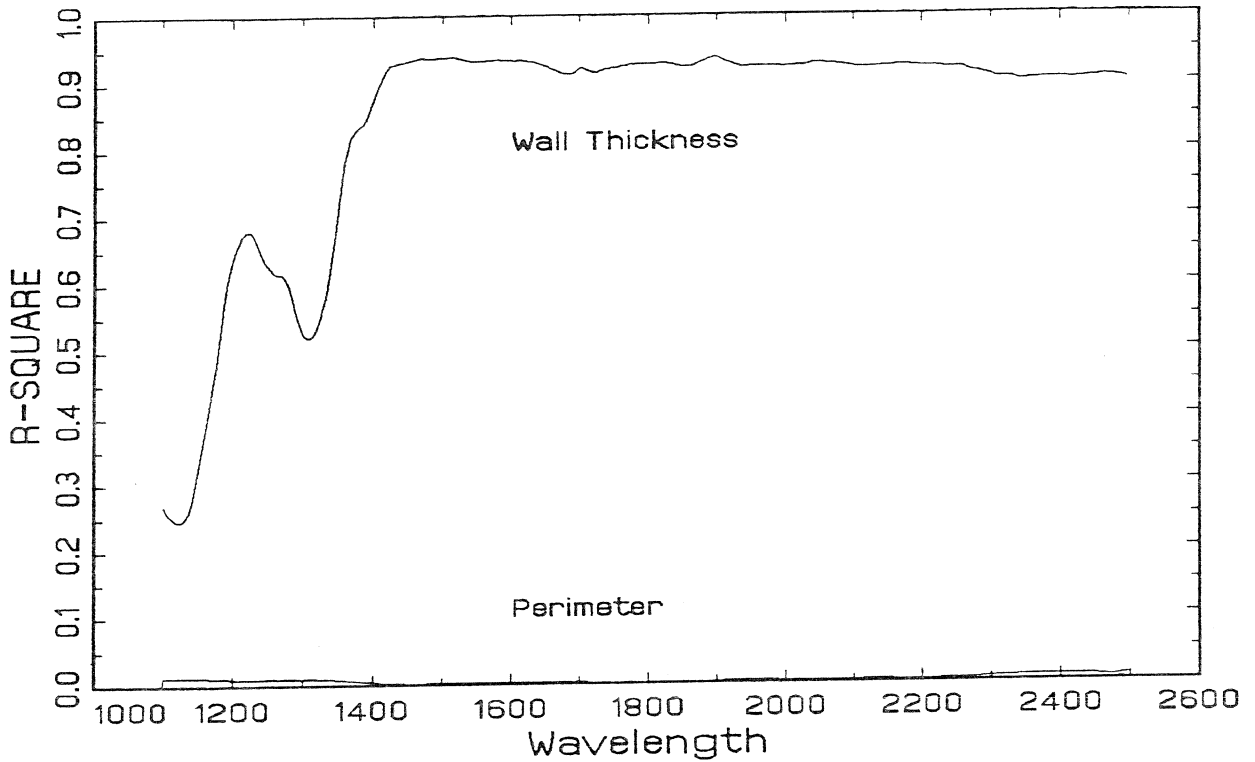
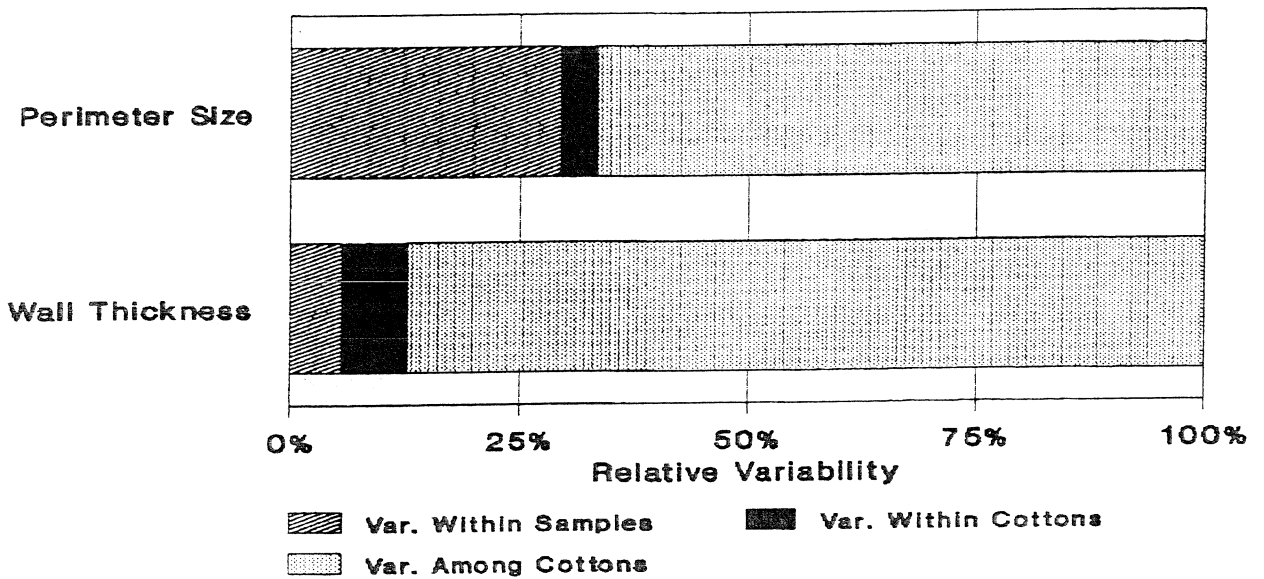


Figure 8. Relative variability of perimeter size and wall thickness as measured by the Arealometer.



101 Cottons
 2 Samples per Cotton
 2-3 Determinations per Sample