COTTON FIBER QUALITY CHARACTERIZATION WITH VIS-NIR REFLECTANCE SPECTROSCOPY: TOWARD AN OPTIMAL SENSOR

Yufeng Ge
J. Alex Thomasson
Biological & Agricultural Engineering Department - Texas A&M University
College Station, TX
Ruixiu Sui
USDA – ARS Cotton Ginning Research Unit
Stoneville, MS

Abstract

The objectives of this research are to (1) assess the performance of the Vis-NIR method for predicting cotton fiber quality parameters with different calibration methods, and (2) determine useful spectral wavebands and bandwidths for predicting various fiber quality parameters. This study is directed toward the development of optoelectronic sensors to measure cotton fiber quality in real time in situ. Sixty seed cotton samples of two varieties were handpicked and ginned with a laboratory-scale saw-type gin. Ginned lint samples were measured with a Cary 500 UV-Vis-NIR spectrophotometer in a wavelength range from 400 to 2500 nm. A portion of the lint samples was subjected to High Volume Instrument (HVI) measurement of six fiber quality parameters: micronaire, length, strength, uniformity, brightness (Rd), and yellowness (+b). Two methods, band-averaging (BA) and discrete wavelet transform (DWT), were used to preprocess the spectral data. Calibration models for each fiber quality parameter were developed with multiple linear regression (MLR) and partial least squares regression (PLSR); and the performance of the models was assessed with cross validated root mean squared error ($RMSE_{cv}$) and coefficient of determination (R^2) between predicted and measured values. Among all six fiber quality parameters, micronaire and +b can be most successfully predicted, with R^2 greater than 0.80 and 0.70, respectively. Prediction of length, uniformity, and strength was moderately successful, with R^2 ranging from 0.40 to 0.70. Prediction of Rd was poor ($R^2 < 0.4$). More interestingly, the $RMSE_{cv}$ of the calibration model for most fiber quality properties approaches the measurement accuracy of HVI instruments specified by USDA-AMS, indicating that a Vis-NIR optoelectronic sensor could perform with an acceptable level of measurement accuracy. Among the different model calibration methods, DWT-MLR generally performed better than BA-MLR and BA-PLSR, which can be attributed to the fact that DWT considers wavebands of varying bandwidths for incorporation into the model. Results of this study indicated that development of optoelectronic sensors based on Vis-NIR reflectance of cotton lint appears promising.

Introduction

Cotton fiber quality is a very important factor throughout cotton research, production, processing, and consumption. Breeders want to develop genetic lines that give rise to superior lint quality. Producers and ginners want to maintain high-quality fibers through advanced harvesting and ginning technologies so that the economic value of cotton can be maximized. Cotton of specific quality is also anticipated by textile processors as it will improve the efficiency of spinning and quality of dyeing. The importance of cotton fiber quality is reflected by the USDA-AMS cotton program, in which virtually every bale of cotton produced in the U.S. is subjected to mandatory High Volume Instrument (HVI) classing. Bales of higher quality are awarded premiums, whereas those of poorer quality are penalized with discounts. Marketing is another factor that exerts a lot of pressure on the U.S. cotton industry. As the largest cotton exporter in the world, U.S. cotton receives criticism about its quality, primarily due to the high degree of machine-cotton interaction through harvesting and ginning (Delta Farm Press, 2004). It is therefore imperative to maintain or even enhance the quality of U.S. cotton so that its competitiveness in the international market can be retained.

Two systems currently used for cotton fiber quality measurement and classification are HVI and Advance Fiber Information System (AFIS). HVI is fully commercialized, and is authorized by the USDA-AMS for classifying U.S. cotton for domestic and international use. HVI reports several bulk fiber quality parameters including color and leaf grades, micronaire, fiber length, strength, uniformity, etc. AFIS requires a lesser volume of fibers to be tested, and it measures additional fiber quality parameters (e.g., short fiber content and nep counts) that are especially important to understand fiber damages during machine-fiber interaction. Microscopic imagery has also been proposed for fiber quality analysis (Xu and Huang, 2004). This method can precisely depict individual fiber cross sections. However, it is very labor intensive and time consuming, and it has difficulty being represented of bulk cotton fibers because of the necessarily small number of fibers involved in the analysis.

The literature suggests that visible and near infrared (Vis-NIR) reflectance spectroscopy could be a useful tool for cotton fiber quality measurement. The line of research conducted by Montalvo and colleagues (Montalvo 1991; Montalvo et al., 1993; Montalvo and VonHoven, 2004; Rodgers et al., 2009) showed that NIR reflectance could satisfactorily predict micronaire, maturity, and fineness. Another independent line of research conducted by Thomasson and colleagues (Thomasson et al., 1995; Wang, 2004; Sui et al., 2008) also verified that fiber diffuse reflectance at the Vis-NIR-MIR region can be used to predict micronaire and other fiber characteristics. Compared to HVI and AFIS, the Vis-NIR method has many advantages. First, it is non-destructive and flexible, and requires minimum sample preparation. This makes real-time in-situ analysis of cotton fiber quality possible. Once the calibration models are built, a single Vis-NIR scan can give measurement for many fiber quality parameters. This would significantly improve the efficiency of measurement. It is also conceivable that a rugged, filter-wheel based optoelectronic sensor can be developed based on Vis-NIR. Such a sensor could be installed on a cotton harvester for real-time fiber quality mapping, in a gin or textile mill for ginning or blending process control. Such a sensor would also support many fiber quality research areas (such as in plant breeding and agronomy) by providing effective, rapid, and non-destructive means for fiber assessment. The very first step toward such an optoelectronic sensor is to identify the most informational bands in the Vis-NIR spectral region so that proper optical and electronic components (e.g., filters and detectors) can be identified.

The long term goal of this study is to develop optoelectronic sensors that can measure cotton fiber quality under various circumstances. Toward that end, the specific research objectives are to (1) assess and compare the performance of various Vis-NIR methods for predicting cotton fiber quality parameters, and (2) determine useful spectral bands and bandwidths for predicting the fiber quality parameters.

Materials and Methods

Sixty cotton samples were used in this study. These cotton samples were hand harvested from two cotton fields on the Texas AgriLife Research Farm in Burleson County, TX. Thirty six samples belong to the variety DPL 164 B2RF (Delta Pine & Land Company, Scott, Miss.) and the remaining 24 belong to the variety DPL 161 B2RF. Hand harvested seed cotton samples were ginned with a laboratory scale saw gin at Texas A&M University's Cotton Improvement Lab. Two subsamples were obtained from each lint sample. One full set of subsamples was used for spectral reflectance measurement. The other subsample set was sent to the Fiber and Biopolymer Research Institute (Lubbock, Texas) for HVI fiber quality determination as the reference measurement for Vis-NIR model development. In this paper we focused on six fiber quality parameters: micronaire, fiber length, length uniformity, fiber strength, reflectance (Rd), and yellowness (+b).

A Cary 500 UV-Vis-NIR spectrophotometer (Varian, Inc., Palo Alto, CA) was used for reflectance measurements, in a wavelength range from 400 to 2500 nm with a spectral sampling interval of 1 nm. Lint cotton samples were placed in a plastic sample holder with an optical window, which was then pressed against the spectrophotometer's scanning entry port for spectral measurement. The window of the sample holder was made of sapphire glass (1-mm thick), which has constant optical transmission in the wavelengths from 400 to 2500 nm. White referencing was done by using a manufacture provided polytetrafluoroethylene disk placed behind a piece of sapphire glass having the same thickness as the optical window of the sample holder.

The cotton spectral data were preprocessed with two different methods to improve the signal to noise ratio and reduce the dimensionality of data for effective model calibration. The first method was to average reference spectra at 20 nm increments. This reduces the number of data points of each spectrum from 2100 to 105, and the nominal wavelengths of these averaged bands are 410, 430… and 2490 nm. In the second preprocessing method, the spectral data were subjected to discrete wavelet transform (DWT). Wavelet coefficients at higher scales (having a support smaller than 16 nm) were discarded since they were usually associated with transient noise features in the spectrum. Therefore, each cotton spectrum was represented by a set of lower scale wavelet coefficients in the wavelet domain. There have been several studies showing that wavelet analysis can be viably applied to reflectance spectra data and improve the calibration model performance (e.g., Sui et al., 2008; and Viscarra Rossel and Lark, 2009). Readers are referred to Ge et al. (2007) for details on the mathematical background of DWT. One big advantage of using DWT is that it results in wavelet regressors that cover varying spectral bandwidths (in contrast to band averaging that gives a constant bandwidth). From a sensor development point of view, this grants researchers a lot of flexibilities in choosing optical filters of varying FWHM (full width at half maximum, an instrumentation terminology similar to bandwidth) at different central wavelengths.

Multiple linear regression (MLR) with the stepwise variable selection criterion was used to develop Vis-NIR calibration models for the six HVI fiber quality parameters. MLR was performed on both 20-nm averaged and wavelet transformed spectra. Partial least square regression (PLSR), which is considered by many as a standard chemometric method, was also applied to 20-nm averaged spectra. Root mean squared error of cross validation ($RMSE_{cv}$) and coefficient of determination (R^2) between predicted and measured values were used to evaluate the performance of each Vis-NIR calibration model. $RMSE_{cv}$ was calculated as follows.

$$RMSE_{cv} = \sqrt{\frac{\sum_{N}(Y_{pred} - Y_{mea})^2}{N}} \quad (1)$$

where N is the number of samples (in this study N = 60); Y_{pred} is the predicted fiber quality parameter with leave one out cross validation; and Y_{mea} is the measured fiber quality parameter with the reference HVI method.

PLSR modeling was performed in R statistical software (R Development Core Team). DWT of cotton reflectance spectra and stepwise MLR were performed with MATLAB's wavelet and statistics toolbox, respectively.

Results and Discussion

Table 1 gives the summary statistics of the HVI fiber quality parameters of 60 lint cotton samples in this study. Because the cotton samples were collected from two fields located very close to one another, the degree of variation for all six cotton fiber quality parameters was relatively small (largely in-field variation). The highest level of variability was exhibited by micronaire and +b (CV = 12.8 and 12.1, respectively). Ideally we would want the cotton samples to be as diverse as possible so that the Vis-NIR calibration models would not be dependent on certain conditions (e.g., variety, harvest method). This issue will be addressed in future work by including very diverse samples (with respect to variety, growing condition, harvest/ginning method) into Vis-NIR model calibration.

Table 1. Summary statistics of the fiber quality parameters of 60 lint cotton samples measured by High Volume Instrument as the reference method for Vis-NIR model calibration.

Fiber quality parameters	Min.	Mean	Median	Max.	SD	CV (%)
Micronaire	2.96	4.05	4.01	4.95	0.52	12.8
Length (in.)	1.08	1.19	1.19	1.26	0.05	4.2
Strength (g tex^{-1})	23.5	28.5	28.9	32.3	2.2	7.9
Uniformity (%)	79.9	83.2	83.4	85.6	1.3	1.7
Rd	67.2	70.5	70.3	74.6	1.7	2.4
+b	6.2	8.1	8.3	9.8	1.0	12.1

The Vis-NIR calibration models with band-averaging and MLR are summarized in table 2. Among the six fiber quality parameters, micronaire and +b can be predicted fairly well, with R^2 values of 0.88 and 0.79. Moderate prediction accuracy is achieved for length, strength, and uniformity (R^2 values greater than 0.55 but less than 0.70). Prediction of Rd is poor (R^2 equals 0.25). Different numbers of spectral bands were included in the calibration models for different quality parameters. For example, the model for micronaire has six spectral bands whereas the model for strength has only two. If an optoelectronic sensor for micronaire were developed, it would require six optical filters with central wavelengths as specified in table 2 (all would have an FWHM of 20 nm). In general, different quality parameters had different informational bands, though some common bands were found among different parameters (e.g., 410 for strength, uniformity, and +b).

Table 2. Leave-one-out cross validation results of the Vis-NIR prediction models for six High Volume Instrument fiber quality parameters. Twenty-nanometer averaged reflectance data were used as the predictor variables; and bands were selected using multiple linear regression with the stepwise variable selection criterion.

Fiber quality parameters	No. of wavebands	R^2	$RMSE_{cv}$	Central wavelengths of selected wavebands (nm)
Micronaire	6	0.88	0.18	430, 1470, 1590, 1650, 2070, 2230
Length (in.)	5	0.66	0.029	530, 670, 1090, 1350, 1470
Strength (g tex^{-1})	2	0.56	1.49	410, 1750
Uniformity	4	0.63	0.89	410, 730, 2070, 2230
Rd	1	0.25	1.45	430
+b	4	0.79	0.45	410, 790, 810, 1750

The Vis-NIR calibration models with DWT and MLR are summarized in table 3. Compared to band-averaging, DWT improved the model accuracy for all quality parameters (except for micronaire, which had a slight decrease in R^2). The largest improvements were in Rd and strength (R^2 increased from 0.25 to 0.39 and 0.56 to 0.66, respectively). It should be noted that due to the multi-resolution capability of DWT, the informational bands included into the model have varying bandwidths. In addition to improved accuracy, another advantage of DWT is that it generally leads to a fewer number of bands in the model (except for Rd). This would subsequently lead to a simpler sensor design (i.e., requiring fewer optical filters). For instance, if a sensor were developed for micronaire, only four (table 3) optical filters are needed instead of six (table 2) as determined by the band averaging method.

Table 3. Leave-one-out cross validation results of the Vis-NIR prediction models for six High Volume Instrument fiber quality parameters. Spectral data were wavelet transformed and then used as the predictor variables; and bands were selected using multiple linear regression with the stepwise variable selection criterion. Bandwidth information for each selected band was given in bracket.

Fiber quality parameters	No. of wavebands	R^2	$RMSE_{cv}$	Central wavelengths of selected wavebands (nm)
Micronaire	4	0.86	0.19	590 [128], 704[32], 1632[32], 1976[16]
Length (in.)	4	0.70	0.027	448 [32], 590 [128], 950 [64], 1384 [16]
Strength (g tex^{-1})	2	0.66	1.30	544 [32], 590 [128]
Uniformity	3	0.68	0.77	560 [64], 1112 [16], 1928 [16]
Rd	2	0.39	1.30	1640 [16], 2136 [16]
+b	2	0.81	0.42	590 [128], 1496 [16]

Figure 1 compares three different calibration methods used in this study. PLSR's performance was poorer than the other two methods. A possible explanation is that PLSR tends to include all available bands (in this case, 105 20-nm averaged bands) into the calibration models. Many of these bands do not contain pertinent information for the fiber quality parameters. Their inclusion therefore tends to introduce noise into the models that would decrease their prediction accuracy.

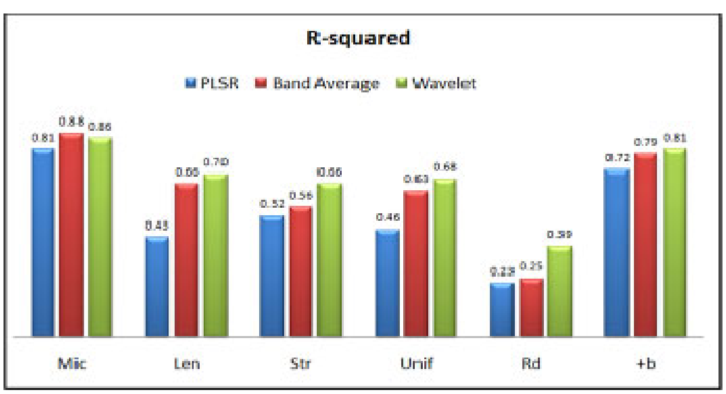

Figure 1. Comparison of three different model calibration methods for six cotton fiber quality parameters.

Table 4 compares $RMSE_{cv}$ of the Vis-NIR prediction model (obtained with the DWT and MLR method) and the accuracy of the reference HVI measurement as specified by the USDA-AMS (USDA, 2001). For some fiber quality parameters (strength, uniformity, and +b), $RMSE_{cv}$ is lower than the accuracy value of HVI. For others (micronaire, length, and Rd), $RMSE_{cv}$ is higher but within a comparable range. Since RMSE can be regarded as the mean deviation of predicted values from the reference values (or true values), this suggests that the accuracy of Vis-NIR can approach that of the reference HVI method. Vis-NIR can therefore potentially be a very important tool for cotton fiber quality measurement.

Table 4. Comparison of $RMSE_{cv}$ obtained with the discrete wavelet transform and multiple linear regression method and the accuracy of reference High Volume Instrument measurement as specified by the USDA-AMS.

Fiber quality parameters	Accuracy	$RMSE_{cv}$
Micronaire	± 0.150	0.190
Length (in.)	± 0.018	0.027
Strength (g tex^{-1})	± 1.500	1.303
Uniformity	± 1.200	0.772
Rd	± 1.000	1.300
+b	± 0.500	0.421

Summary and Conclusions

The long term goal of this study is to develop optoelectronic sensors to measure cotton fiber quality real time in situ. The specific objectives were to: (1) assess the performance of the Vis-NIR method for predicting cotton fiber quality parameters with different calibration methods, and (2) determine useful spectral bands and bandwidths for predicting various fiber quality parameters. Sixty seed cotton samples of two varieties were handpicked and ginned with a laboratory-scale saw-type gin. Ginned lint samples were measured with a Cary 500 UV-Vis-NIR spectrophotometer in a wavelength range from 400 to 2500 nm. A portion of the lint samples was subjected to HVI measurement of six fiber quality parameters: micronaire, length, strength, uniformity, Rd, and yellowness (+b). Two methods, band averaging and DWT, were used to preprocess the spectral data. Calibration models for each fiber quality parameter were developed with MLR and PLSR; and the performance of the models was assessed with $RMSE_{cv}$ and R^2 between predicted and measured values. The results showed that the best prediction accuracy was achieved for micronaire and +b ($R^2 > 0.70$), followed by length, uniformity, and strength ($R^2 > 0.40$). Prediction of Rd was not successful ($R^2 < 0.40$), but the reason is not known at the time of this writing. Comparing the three prediction methods, DWT with MLR give the best results. This fact may be attributed to the multi-resolution capability of DWT. The $RMSE_{cv}$ value of the DTW with MLR method for all fiber quality parameters is comparable to the measurement accuracy of the reference HVI method as specified by the USDA-AMS. Development of optoelectronic sensors based on Vis-NIR reflectance of cotton lint, particularly with band selection based on DWT with MLR, appears promising.

Acknowledgements

We would like to thank Mr. Scott Stanislav for handpicking cotton samples and Texas AgriLife Research's Cropping Systems Program for providing funding for this project.

References

Delta Farm Press. 2004. Many problems: China critical of U.S. cotton quality.

Ge, Y., C.L.S. Morgan, J.A. Thomasson, T. Waiser. 2007. A new perspective to near-infrared reflectance spectroscopy: A wavelet approach. Trans. ASABE 50:303–311.

Montalvo, J.G., Jr. 1991. A comparative study of NIR diffuse reflectance of cottons grouped according to fiber cross-sectional dimensions. Part I: Fundamentals. Applied Spectroscopy 45:779-789.

Montalvo, J.G., Jr., S.E. Faught, H.H. Ramey, Jr., and S.E. Buco. 1993. Studies to measure cotton fibre length, strength, micronaire and colour by vis/NIR reflectance spectroscopy. Part I: Descriptive statistics of fibre properties and reflectance spectra. Journal of Near Infrared Spectroscopy 1:153–173.

Montalvo, J.G., and T.M. VonHoven. 2004. Update on micronaire, maturity and fineness research. In proceedings of 2004 Beltwide Cotton Conferences p. 2342-2349. Jan 5-9. San Antonio, TX. National Cotton Council of American.

Rodgers, J., J. Montalvo, G. Davidonis, and T. VonHoven. 2009. Near infrared measurement of cotton fiber micronaire, maturity and fineness – a comparative investigation. Textile Research Journal 0:1–14.

Sui, R., J.A. Thomasson, Y. Ge, and C. Morgan. 2008. Multispectral sensor for in-situ cotton fiber quality measurement. Trans. ASABE 51:2201–2208.

Thomasson, J.A., and S.A. Shearer. 1995. Correlation of NIR data with cotton quality characteristics. Trans. ASAE 38:1005–1010.

USDA. 2001. The Classification of Cotton. Agricultural Handbook 566. Washington, D.C. 20250.

Viscarra Rossel, R.V., and R.M. Lark. 2009. Improved analysis and modeling of soil diffuse reflectance spectra using wavelets. European Journal of Soil Science 60:453–464.

Wang, R. 2004. Site-specific Prediction and Measurement of Cotton Fiber Quality. Unpublished Dissertation. Department of Agricultural and Biological Engineering, Mississippi State University. Mississippi State, MS.

Xu, B., and Y. Huang. 2004. Image analysis of cotton fibers part II: Cross-sectional measurements. Textile Research Journal 74:409–416.