TEXTILE TECHNOLOGY

Near-Infrared Classification of Cotton Lint, Botanical and Field Trash

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ABSTRACT

It is advantageous to produce cotton of the highest quality while minimizing the effect and presence of trash within the cotton lint. In addition, cotton trash comingled with the lint adversely affects the quality and profit margin associated with producing, harvesting, and processing cotton. The popularity of High Volume Instrumentation (HVITM) has spread because it provides instrument-based cotton quality measurements (e.g. length, strength, length uniformity, micronaire, color, and trash content). However, this instrument does not specifically determine the types of trash present within the lint. Software was utilized to determine the specific identity of various pure samples of botanical and field trash types using Near-Infrared (NIR) spectroscopy. Results of this study reveal that NIR spectroscopy identified 100% homogeneous individual samples of botanical trash yielding an overall accuracy of 98% for the combination of botanical and field trash.

Lower quantities of trash in harvested cotton decreases the need for lint cleaning treatment thus affecting profit margins for cotton producers and enhancing the overall cotton quality for yarn and fabric formation. The creation of quality measurements must enhance the value of cotton using a method that is accurate, precise, and fast.

Cotton lint becomes comingled with foreign matter during cotton harvesting and ginning. Complicating this problem is the tendency of cotton trash to become much smaller in size during its processing, making cotton trash identification difficult. Earlier reports have implicated cotton trash in yarn breakage (Brashears et al., 1992), rotor spinning deposits (Foulk et al., 2004), and mechanical nep formation (Frey and Schneider, 1989).

Presently, HVITM is widely used to measure cotton quality parameters such as micronaire, length, strength, length uniformity, color, and trash content (Uster Technologies, Knoxville, TN). The HVITM uses a visible imaging technique in which trash particle count and area are used to define the amount of trash present in a sample. However, one limitation of using the HVITM method is the lack of specificity in the identification of individual trash botanical components such as the hull, leaf, seed coat, seed meat, and stem as well as other contamination.

In contrast to HVITM grading, the Shirley Analyzer determines trash content via a gravimetric technique using aero-mechanical separation of cotton fiber from trash (ASTM, 2007). The Shirley Analyzer also does not specify cotton trash types. Previous classification of cotton trash employed cluster analysis, neural networks, and visible image analysis (Siddaiah et al., 2006; Siddaiah et al., 2009; Whitelock et al., 2009; Xu et al., 1999). Himmelsbach et al. (2006) successfully utilized Mid-Infrared (MIR) spectroscopy to evaluate cotton and grass botanical parts, sugars, synthetic materials (e.g. woven bale wrap, plastic shopping bag, bale strapping), inorganic and organic materials . An Attenuated Total Reflectance (ATR) accessory was able to identify cotton trash types that led to the creation of an MIR spectral library.

The NIR spectral region encompasses 800 to 2500 nm (4000 to 12500 cm^{-1}) where the regions are defined as first, second, and third overtones or combination bands (Burns, 1985). Primarily, the NIR spectral region encompasses 1100 to 2500 nm. Primary absorbencies observed in the NIR spectral region are the chemical species CH_i, NH_i, and OH (Rodgers, 2002). Similar to HVI for trash measurements, NIR spectroscopy offers many advantageous features including little to no sample preparation, non-destruction of samples, and ease of use. In addition, NIR spectroscopy also allows flexibility of multiple sampling systems (e.g. fiber optic probe, rotating sphere); and the option of analyzing powder-size, pepper-size, and raw trash samples (e.g. "sticks"), (Rodgers, 2010a, 2010b). Based on these characteristics, NIR has been previ-

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ously used to study textiles, including cotton (Camjani and Muller, 1996; Montalvo et al., 1991; Montalvo and von Hoven, 2004; Rodgers, 2002; Rodgers and Beck, 2005, 2009; Rodgers and Ghosh, 2008; Rodgers et al., 2010a, 2010c; Taylor, 1980; Thibodeaux, 1992; Thomasson and Shearer, 1995).

Identification of cotton trash has been attempted using NIR (Taylor, 1996). However, this technique was complicated by small levels of trash particle contrast between bark and grass making identification of trash components difficult. In a recent preliminary study, an NIR spectral library was employed to accurately classify and identify specific botanical cotton trash types (Fortier et al., 2010). The goal of this study was to improve an existing NIR spectral library based on different botanical trash types by including seed meat and pure samples of field trash.

MATERIALS AND METHODS

Cotton and Cotton Trash Samples. The NIR spectral library and the prediction set consisted of one class of "clean" cotton used as the cotton reference, and 35 powder-sized (0.177 mm std. diameter) and pepper-sized (0.841 mm std. diameter) trash samples of 9 botanical cotton trash sources denoted by the first two letters from the state the samples were acquired in and the last letter as the sample variety (MSA = Mississippi DP555, NMA = New Mexico DP555, NMB = New Mexico Acala 1517-99, NMC = New Mexico Unknown, SCA = South Carolina DP458, SCB = South Carolina DP555, SCC = South Carolina DP555a (second sample), SCD = South Carolina FM989, and SCE = South Carolina PM1218. In addition, field trash

Table 1. Calibration set of cotton trash sa	mples
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including 1) grocery bag, blue module cover, black plastic bag, clear plastic bag, and white module cover (all composed of polyethylene) and 2) module cover strap and twine (both composed of polypropylene) were added to the spectral library. The Bruker OPUS IDENT software was used to create the NIR spectral library. Botanical trash types for the powder- and pepper-sized samples and raw seed meat samples were identified by 1) assigning the first two letters of the state the samples were produced in (either Mississippi (MS), New Mexico (NM), or South Carolina (SC)) and 2) assigning the last letter to denote the pure trash variety (see Table 1). A total of 39 averaged samples based on three replicates for the powder- and pepper-sized trash types along with raw seed meat samples were used as the calibration set. For the prediction set, a total of 114 individual samples of powder-, and pepper-sized trash samples and raw seed meat samples of different varieties were used to validate the method. There were 9 raw seed meat samples, 5 of which were included in the calibration set (to make the calibration set more robust), as shown in Table 1, and the remaining 4 different raw seed meat samples were included in the prediction set. The hull, leaf, seed coat, seed meat, and stem group samples were used to develop the spectral library. The calibration set spectral library was then expanded to include some types of field trash (grocery bag, black plastic bag, blue module cover, clear plastic bag, module cover strap, twine, and white module cover). Two replicate measurements were included for each individual field trash sample type in the calibration and prediction set. Thus, 14 samples of field trash were included in the calibration set and 14 samples of field trash were included in the prediction set.

Cotton Trash Variety and Size		Trash Types		
MSA (powder)	Hull	Leaf	Seed Coat	Stem
NMA (pepper)	Hull	Leaf	NS	Stem
NMB (powder)	Hull	Leaf	Seed Coat	Stem
NMC (pepper)	Hull	Leaf	Seed Coat	Stem
SCA (pepper)	Hull	Leaf	Seed Coat	Stem
SCB (powder)	Hull	Leaf	Seed Coat	Stem
SCC (pepper)	Hull	NS	Seed Coat	Stem
SCD (pepper)	Hull	Leaf	Seed Coat	Stem
SCE (powder)	Hull	Leaf	Seed Coat	Stem
MSA, NMB,NMA,NMC,SCA	Raw seed meat			

NS = no sample. (The cotton trash varieties are denoted by the first two letters from the state the samples were acquired in and the last letter as the sample variety (MSA = Mississippi DP555, NMA = New Mexico DP555, NMB = New Mexico Acala 1517-99, NMC = New Mexico Unknown, SCA = South Carolina DP458, SCB = South Carolina DP555, SCC = South Carolina DP555a, SCD = South Carolina FM989, SCE = South Carolina PM1218). **NIR spectroscopy.** The NIR spectra were acquired using a bench top Bruker MPA instrument fitted with a solid fiber optic probe (Bruker Optics, Billerica, MA). Near-Infrared data acquisitions were acquired by putting the pure trash samples in direct contact with the solid probe head, which has a diameter of 3mm. Three replicate spectra were acquired at a resolution of 8 cm⁻¹ and 128 scans for the "clean" reference cotton lint and each pure trash component. Specific frequency/wavelength regions were investigated to cover the entire spectral range 800 to 2500 nm (4000 to 12500 cm⁻¹).

NIR OPUS IDENT software. Near-Infrared absorbance spectra were analyzed using the Bruker OPUS IDENT software package. In this software package, the spectral types were separated into groups representing the cotton, botanical trash and field trash. Preprocessing methods such as vector normalization, first derivative, and vector normalization with first derivative were investigated to normalize the spectral data (Optics, 2009). In addition, mathematical algorithms including the standard method and factorization were used to develop the identification models. Specific frequency/wavelength regions (1100 to 2400 nm, 1427 to 1867 nm, 1100 to 1800/2000 to 2400 nm) were investigated to cover the entire spectral range and select spectral ranges, such as those with and without moisture peaks.

RESULTS AND DISCUSSION

NIR Spectral Library Development. In the development of the NIR reference library, it was necessary to include spectra from numerous sources to make the qualitative method robust. Threshold values were calculated for each group (cotton and individual trash components). These threshold values were calculated based on statistical measurements of the spectra. These statistical measurements, including calculating the Euclidean distances, were aimed at limiting the variability between reference spectra of different groups while capitalizing on the similarities which existed between spectra in a specific group. The Euclidean distance was a measure of the similarity between reference spectra of a specific group in the library. In effect, calculating the Euclidean distances set up the confidence limit of the threshold values. If the individual reference spectra were below the confidence limit of the average reference spectra for a certain group ("hit quality"), the individual spectrum was said to be a

member of that group. After the thresholds were determined for each respective group in the library, validating the library was necessary to determine how well the library members are separated. After all of the reference library component groups were uniquely identified, the library was saved. Unknown spectra were evaluated with the saved library and the identity of the unknown spectra was determined (Optics, 2009).

Four key parameters were cited on the validation report: the hit number, the hit quality, the threshold value, and the group. The threshold values reported were determined as described earlier and the hit number listed the library groups which were most similar to the unknown spectra in descending order. The hit quality expressed the Euclidean distance from the unknown spectrum to the average reference spectrum in a specific group. The group represents the corresponding group attached to the sample name in the reference library. Unknown spectra having a hit quality value at hit number 1 is determined to be a match with a specific group in the reference library (Optics, 2009).

To optimize setting up the reference library, many pre-processing methods were available to use. The standard method pre-processing, used in many identification routines, calculated the Euclidean distance between the unknown and reference spectra in the spectral library. The factorization pre-processing method calculated the resulting coefficients of the average spectra in the library, which were first represented as a linear combination of factor spectra. The vector normalization pre-processing method first calculated the average y value of spectra and only used data points within the selected spectral ranges. The average value calculated was then subtracted from the spectrum, which caused the spectrum to be centered at around y = 0. This is followed by calculating the sum of squares of all y values, and the respective spectrum was divided by the square root of this sum (Optics, 2009).

Including seed meat in NIR reference library. Originally, a reference library consisting of cotton and pure botanical trash types (hull, leaf, seed coat, and stem) NIR spectra was created to identify cotton and the different botanical trash types as previously described (Fortier e al., 2010). To make this library more robust, seed meat samples were added to this existing library. As can be observed in Figure 1, spectral similarity between NIR absorbance spectra of the trash types was observed, but the seed meat NIR absorbance spectrum is clearly different from the original spectral library components. Vector normalization and the standard method pre-processing were applied over the spectral range of 1100 to 2400 nm. Figure 2 shows the result of applying the first derivative and factorization preprocessing to the spectral library. Again, spectral overlap was observed between the botanical trash types, but the seed meat spectra were clearly spectrally different.

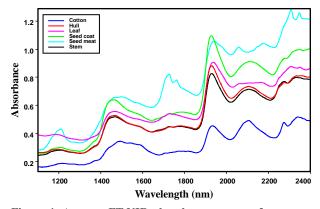


Figure 1. Average FT-NIR absorbance spectra for cotton and pure botanical trash type spectra over entire spectral range (1100-2400 nm). Vector normalization and standard preprocessing was applied.

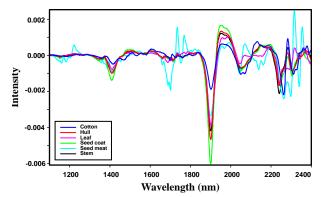


Figure 2. Average FT-NIR spectra for cotton and botanical trash types over entire spectral range (1100-2400 nm). First derivative with standard preprocessing was applied.

As can be observed in Figures 1 and 2, all of the trash samples have spectral bands at 1720 nm representing the (C-H) first overtone asymmetrical stretch, and a band at 1459 nm representing an (O-H) stretch first overtone (Burns et al., 2008). Both the cotton and trash types have a band at 1930 nm. Previous investigations have shown that the 1930 nm band is due primarily to water (Rodgers et al., 2010a). Cotton has distinct bands from 1215 nm to 1225 nm representing the (C-H) second overtone, a band at 1370 nm representing a (C-H) combination, a band at 1590 nm representing (O-H) first overtone (intramolecular hydrogen bond), and a band at 1702 nm representing the (C-H) stretch first overtone (Burns et al., 2008). The leaf trash has a unique band at 1695 nm representing the (C-H) stretch first overtone. Both leaf and seed meat trash types have a spectral band at 2310 nm, representing the (C-H) band second overtone (Beck, 1996). For the seed meat trash, it has distinctive spectral bands at 1757 nm representing the (C-H) first overtone, a band at 2174 nm representing the asymmetrical (C-H) stretch/(C-H) deformation combination, and a band at 2304 nm representing the (C-H) second overtone (Burns et al., 2008). Two bands representing cotton and cotton botanical trash, with the exception of leaf and seed meat, are observed at 2100 nm with an (O-H) bend and C-O stretch combination and a band at 2270 nm representing O-H bend and C-O stretch combination/C-H stretch and CH₂ deformation (Shenk et al., 2008; Beck, 1996).

After iteration with different spectral ranges and preprocessing techniques, seed meat spectra were added to the original library over the spectral ranges of 2284.2 to 2400.4 nm, 1920.4 to 2174.9 nm, and 1426.1 to 1869.1 nm creating a complete distinction between cotton, leaf, seed meat and stem with first derivative, vector normalization, and factorization preprocessing. A sub-library was then created to distinguish between hull and seed coat over the spectral range of 2284.2 to 2400.4 nm with first derivative and factorization preprocessing. The necessity of creating the sub-library was not surprising since this step was required in the original library without seed meat (Fortier et al., 2010). Adding seed meat to the original library gave an overall accuracy of 97.37% as shown in Table 2. The separation of all of the components under these conditions can be observed with the score plot in Figure 3.

 Table 2. NIR Prediction Set Identification by Cotton Trash

 Type for Individual Powder and Pepper samples adding

 seed meat to the original library.

Prediction Set	Individual Powder and Pepper Samples ^a		
Trash Type	% Correct	Number of samples	Number Correct
Hull	100%	27	27
Leaf	100%	27	27
Seed Coat	90.48%	21	19
Seed Meat	100%	12	12
Stem	96.30%	27	26
Total	97.37%	114	111

%Correct = (No. Correct/No. of samples)*100

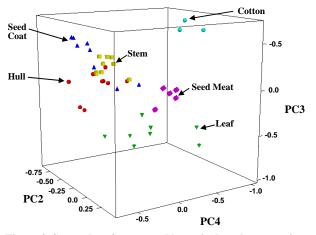


Figure 3. Score plot of cotton and botanical trash types using the "top down" approach.

Since the seed meat spectra were so distinctly different from other cotton and cotton botanical trash spectra and basically flooded the spectral library, the "top down" approach was used to improve the identification of the components in the spectral library with the addition of seed meat. Briefly, a specific spectral range (1206.4 to 1256.7 nm) and first derivative and factorization preprocessing method was chosen to first isolate seed meat from the other components in the original library. Next, the remaining components (hull, leaf, seed coat, stem and cotton) were included in a sub-library to be spectrally distinguished over the spectral range of 1426.8 to 1867.8 nm, and first derivative and factorization preprocessing. This step separated cotton, leaf, and stem trash types. Finally, a second sub-library was created to separate the hull and seed coat trash types. As was carried out before with the original library, the spectral similarity between the hull and seed coat required the formation of a sub-library to distinguish between them. The score plot in Figure 4 shows that this approach was successful at separating and identifying all components in the NIR spectral library. As can be observed from Table 3, the "top down" approach yielded a higher percent accuracy (100% in the correct identification of specific types of botanical trash) compared to adding the seed meat to the original library.

Including field trash in NIR reference library. To expand the utility of the reference library following the inclusion of seed meat, pure field trash samples were added. Field trash including a grocery bag, black plastic bag, blue module cover, clear plastic bag, module cover strap, twine, and white module cover were added to the spectral library over the entire spectral range (1100 to 2400nm) as shown in Figure 5. As can be observed there is some overlap between the blue and black plastic bags, some overlap between the module cover strap and twine, and the grocery bag, clear plastic bag, and white module cover. Given this spectral overlap, the first derivative spectra were investigated for these compounds in the spectral library as depicted in Figure 6 over the entire spectral range of 1100 to 2400 nm.

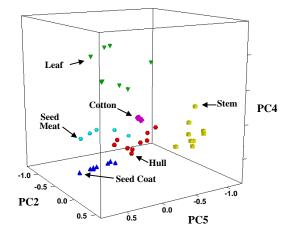


Figure 4. Score plot of cotton and botanical trash types adding seed meat to original NIR library.

Table 3. NIR Prediction Set Identification by Cotton Trash Type for Individual Powder and Pepper samples using the "top down" approach adding seed meat.

Prediction Set	Individual Powder and Pepper Samples ^a		
Trash Type	% Correct	Number of samples	Number Correct
Hull	100%	27	27
Leaf	100%	27	27
Seed Coat	100%	21	21
Seed Meat	100%	12	12
Stem	100%	27	27
Total	100%	114	114

%Correct = (No. Correct/No. of samples)*100

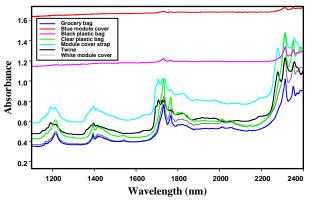


Figure 5. Average FT-NIR absorbance spectra for individual field trash spectra over entire spectral range (1100-2400 nm). No preprocessing and standard method was applied.

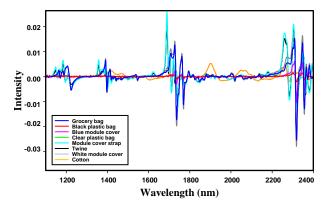


Figure 6. Average FT-NIR spectra for cotton and field trash types over entire spectral range (1100-2400 nm). First derivative with factorization preprocessing was applied.

As can be observed in Figures 5 and 6, the grocery bag, clear plastic bag, and white module cover have some common spectral bands at 1166 nm representing the C-H second overtone asymmetrical stretch, at 1542 nm representing the O-H stretch first overtone (intramolecular hydrogen bond), at 1729 nm asymmetrical methylene (C-H) stretch first overtone, at 1765 nm, (C-H) first overtone, at 2311 nm, representing the (C-H) bend second overtone, and at the 2349 nm band representing the (CH₂) bend second overtone.

The module cover strap and twine field trash groups had common spectral bands at 1150 nm representing the (C-H) second overtone asymmetrical stretch, at 1190 nm representing the asymmetrical (C-H) stretch second overtone, at 1356 nm representing the (C-H) combination stretch and bend, at 1694 nm representing the asymmetrical (C-H) stretch first overtone, at 1704 nm representing the asymmetrical (C-H) stretch first overtone, at 2190 nm representing the (CH2) stretch and bend, at 2278 nm representing the (C-H) stretch and bend, at 2278 nm representing the (C-H) stretch and bend combination, and at 2461 nm representing the (C-H) combination band (Shenk et al., 2008).

The blue module cover and black plastic bag had similar spectral bands to the grocery bag, clear plastic bag, and white module cover at spectral bands 1729, 1765, 2311, and 2349 nm as described earlier, suggesting that all of these pure trash types are composed of polyethylene (Scott and Waterland, 1995). As for the composition of the strap and twine samples, the spectra resemble that of polypropylene (Rodgers and Ghosh, 2008).

Since the field spectra were so distinct and completely different from the botanical trash and cotton spectra and since there was considerable spectral overlap under these conditions, a "top down" approach was applied to the addition of field trash to the spectral library composed of botanical trash. First, pure field trash samples and seed meat were isolated from the rest of the pure botanical trash components over the spectral range of 1314 to 1385.6 nm with factorization. Next, a sub-library composed of cotton, hull, leaf, seed coat, and stem was created with first derivative and factorization preprocessing over the spectral range of 1426 to 1869.1 nm. Finally, a second sub-library was created to separate hull and seed coat spectra over the spectral range of 2284.1 to 2400.4 nm. Under these conditions, 100% of the field trash was accurately identified as shown in Table 4. The score plot shown in Figure 7 indicated distinct separation of the field trash spectra and demonstrated the "tight" grouping of the botanical trash individual components under a "top down" approach to construct a NIR spectral library. Due to the large spectral dissimilarities between the botanical and field trash components, there were a few incorrect assignments in the seed coat and seed meat botanical trash spectral library components. However, when identifying all of the botanical and field trash samples in the prediction set, greater than 98% of the trash types were determined accurately.

Table 4. NIR Prediction Set Identification by Cotton Trash Type for Individual Powder and Pepper samples adding seed meat and field trash using the "top down" approach.

Prediction Set	Individual Powder, Pepper, and Field Trash Samples ^a		
Trash Type	% Number Correct of samples		
Hull	100%	27	27
Leaf	100%	27	27
Seed Coat	95.24%	21	20
Seed Meat	91.67%	12	11
Stem	100%	27	27
Total Botanical Trash	98.25%	114	112
Grocery Bag	100%	2	2
Black Plastic Bag	100%	2	2
Blue Module Cover	100%	2	2
Clear Plastic Bag	100%	2	2
Module Cover Strap	100%	2	2
Twine	100%	2	2
White Module Cover	100%	2	2
Total Field Trash	100%	14	14
Overall Total Trash	98.44%	128	126

%Correct = (No. Correct/No. of samples)*100

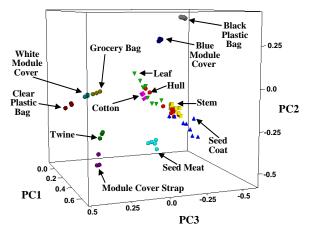


Figure 7. Score plot of NIR library consisting of cotton, botanical and field trash components.

In the current study, it was successfully demonstrated that NIR spectroscopy could be used to specifically define individual botanical and field trash types that can be found in cotton, with an overall 98% accuracy in the identification of the pure botanical and field trash types. The "top down" method where the seed meat was first spectrally isolated from other botanical trash types, gave a higher percent accuracy (100%) for the botanical trash compared to simply adding the seed meat spectra to the existing botanical trash library (97%). Compared to the previously used MIR technique, distinct advantages (e.g., sample size and flexibility of sampling systems) were obtained with the use of NIR. This NIR spectral library has the potential to become even more robust with the inclusion of other trash types and trash mixtures. This technology has the potential to be applied in a commercial cotton trash classification system.

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DISCLAIMER

The use of a company or product name is solely for the purpose of providing specific information and does not imply approval or recommendation by the United States Department of Agriculture to the exclusion of others.

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