# Exploring NIR technique in rapid prediction of cotton trash components

Yongliang Liu, Devron Thibodeaux, and Gary Gamble

Cotton Quality Research Station, ARS, USDA, Clemson, SC 29633

***Abstract:*** Near infrared (NIR) spectroscopy, a useful technique due to the speed, ease of use, and adaptability to on-line or off-line implementation, has been applied to perform the qualitative classification and quantitative prediction on a number of cotton quality indices, including cotton trash from HVI, SA, and AFIS measurement. It is well-known that these current-in-use trash measuring devices only produce the trash values in some aspects, instead of the content for individual trash component. This difficulty comes from the complexity of co-existence of various trash types, for example, leaves (leaf and bract), seed coats, hulls, and stems. Regarding to this, mixtures of known trash components (e.g., leaves, seed coats, hulls, stems, and sand/soil) with cut lint fibers were prepared physically and then their NIR spectra were correlated with the respective trash contents. The results suggested the feasibility of NIR technique in the precise and quantitative determination of total trash, leaf trash and non-leaf trash components.

## 1. Introduction

- Presence of trashes in commercial cotton bales at various amounts degrades the market values and further impacts end-use qualities.
- To ensure a fair trading, the USDA AMS has introduced the high volume instrument (HVI) trash test as a universal standard index. It represents the trash portion only detectable on the surface of a sample.
- In addition, gravimetric-based Shirley analyzer (SA) and advanced fiber information system (AFIS) have also been utilized to determine the trash contents within bulky samples.
- Either HVI or SA or AFIS only yields the amount of trash in general terms, instead of the content for individual trash component.
- Earlier studies revealed poor NIR models on trash contents. Major factor is due to highly diversification of trashes and their heterogeneous distribution.

## 2. Objective

(1) to compare NIR model on individual trash constitute, namely, total trash, leaf trash, non-leaf trash, stem trash, hull trash, seed coat trash, and sand/soil trash.

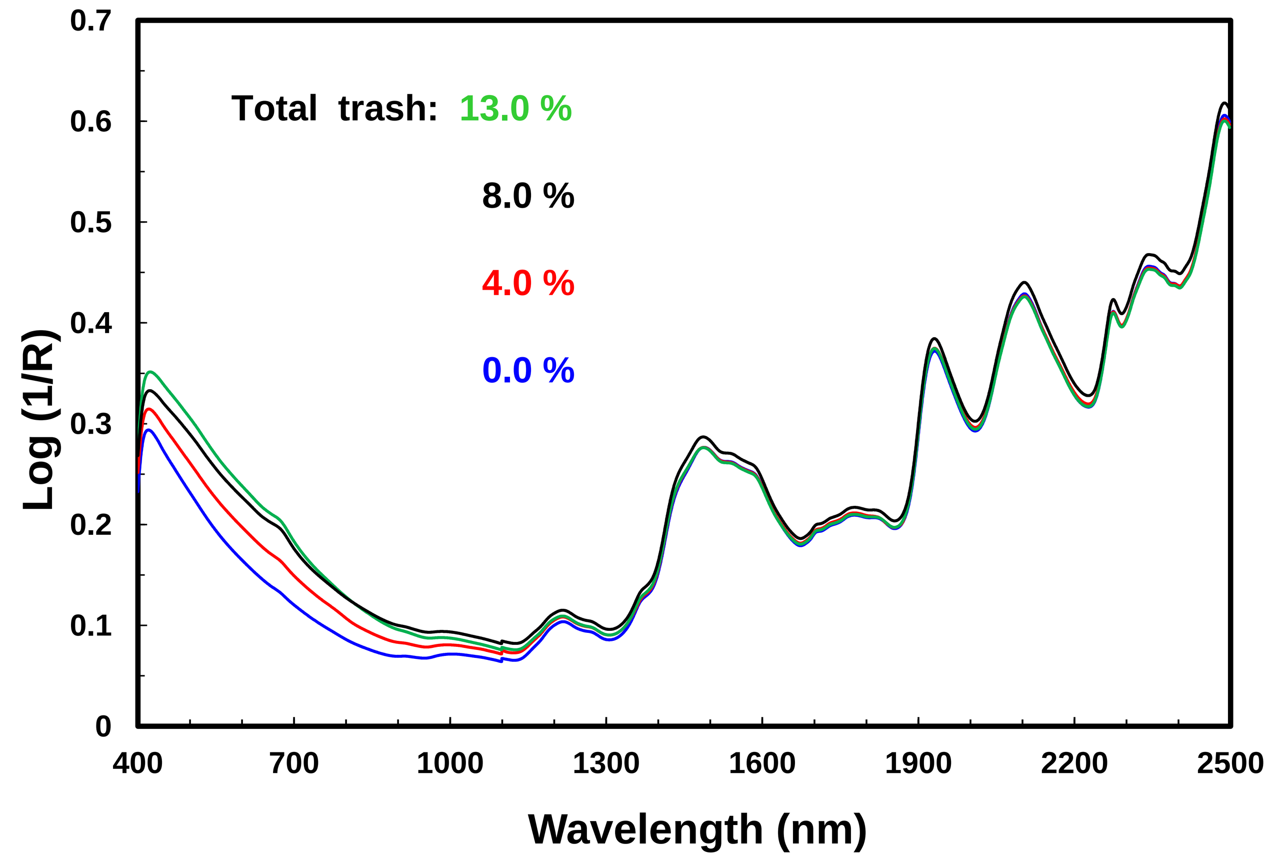
(2) to examine the effect of trash uniformity on NIR model performance.

## 3. Experimental

- **Clean fibers and cotton trashes.** Clean fibers were from Shirley analyzer process, while five types of trashes (leaves/bracts, seed coats, hulls, stems, and sand/soil were collected from 3 varieties of seed cottons in 2008.
- **Ground samples and mixtures.** Both fibers and trashes were grounded in a Wiley mill to pass through a 20-mesh screen. Then 100 mixtures with varying amounts were prepared simply.
- **Visible/NIR reflectance.** Foss XDS spectrometer (400-2500 nm) was used. Mixtures were loaded into a Foss NIR cell (0.38 inch in depth x 2 inch in diameter).
- **Prediction models.** PLSplus/IQ package in Grams/AI (V 7.01, Thermo Fisher Scientific, MA) was utilized to develop models. One third samples were assigned as validations.

## 4. Results and Discussion

### 4.1 Cotton trash contents and visible/NIR spectra




### 4.2 References of individual trash

| Constituent | Calibration (n =67) | | | Validation (n = 33) | | |
|---|---|---|---|---|---|---|
| | Range | Mean | SD | Range | Mean | SD |
| Total trash, % | 0 - 15.0 | 5.08 | 2.83 | 0 - 12.0 | 4.59 | 2.58 |
| leaf trash, % | 0 - 5.0 | 1.40 | 1.05 | 0 - 4.0 | 1.52 | 1.01 |
| non-leaf trash, % | 0 - 12.0 | 3.68 | 2.47 | 0.60 - 9.6 | 3.07 | 2.10 |
| Stem trash, % | 0 - 5.0 | 1.34 | 1.13 | 0 - 4.0 | 1.15 | 0.97 |
| Hull trash, % | 0 - 5.0 | 1.24 | 1.33 | 0 - 3.0 | 0.99 | 0.77 |
| Seed coat trash, % | 0 - 3.0 | 0.61 | 0.77 | 0 - 2.5 | 0.42 | 0.59 |
| Sand / soil trash, % | 0 - 3.0 | 0.50 | 0.73 | 0 - 2.5 | 0.50 | 0.59 |

### 4.3 NIR models on 7 trashes

| Component | Optimal factor | Calibration Set $R^2$ | Calibration Set RMSEC | Validation Set $r^2$ | Validation Set RMSEV | Validation Set RPD |
|---|---|---|---|---|---|---|
| Total trash | | | | | | |
| 405 - 2495 nm | 6 | 0.93 | 0.76 | 0.89 | 0.88 | 2.9 |
| 405 - 1095 nm | 6 | 0.93 | 0.75 | 0.92 | 0.75 | 3.4 |
| 1105 - 2495 nm | 6 | 0.93 | 0.76 | 0.93 | 0.75 | 3.4 |
| 900 - 1700 nm | 6 | 0.94 | 0.69 | 0.92 | 0.72 | 3.6 |
| Leaf trash | | | | | | |
| 405 - 2495 nm | 4 | 0.94 | 0.26 | 0.92 | 0.28 | 3.6 |
| 405 - 1095 nm | 5 | 0.95 | 0.23 | 0.94 | 0.26 | 3.9 |
| 1105 - 2495 nm | 6 | 0.87 | 0.38 | 0.84 | 0.41 | 2.5 |
| 900 - 1700 nm | 8 | 0.89 | 0.35 | 0.89 | 0.35 | 2.9 |
| Non-leaf trash | | | | | | |
| 405 - 2495 nm | 7 | 0.93 | 0.67 | 0.92 | 0.66 | 3.2 |
| 405 - 1095 nm | 6 | 0.91 | 0.73 | 0.90 | 0.68 | 3.1 |
| 1105 - 2495 nm | 7 | 0.95 | 0.54 | 0.91 | 0.69 | 3.0 |
| 900 - 1700 nm | 8 | 0.95 | 0.54 | 0.92 | 0.60 | 3.5 |
| Stem trash | | | | | | |
| 900 - 1700 nm | 7 | 0.78 | 0.53 | 0.65 | 0.59 | 1.6 |
| Hull trash | | | | | | |
| 900 - 1700 nm | 7 | 0.80 | 0.59 | 0.57 | 0.67 | 1.1 |
| Seed coat trash | | | | | | |
| 900 - 1700 nm | 10 | 0.79 | 0.36 | 0.24 | 0.57 | 1.0 |
| Sand/soil trash | | | | | | |
| 900 - 1700 nm | 8 | 0.91 | 0.22 | 0.69 | 0.34 | 1.7 |

* All spectral processing with mean centering (MC) and the first derivative (1st deri.).
* Root mean square error of calibration (RMSEC) and validation (RMSEV).
* RPD = SD / RMSEV.

RPD is often used as a dimensionless gauge of the ability of a spectroscopic model to predict a property:

(i) RPD > 3.0: acceptability for quantitative prediction
(ii) RPD = 3.0 ~ 2.5: suitability for screening application
(iii) RPD < 1.0: lack of modeling power

## 5. Conclusions

- The study demonstrates the feasibility of NIR models for quantitative determinations of total trash, leaf trash and non-leaf trash (RPD = 3.6).
- It indicates the difficulty of NIR in the prediction of such non-leaf trashes as stem, hull, seed coat and sand/soil. This limitation arises from the particle size and their uniform distribution, and further study is necessary.

** We are grateful to M. Morris (ARS, Clemson) for technical assistance in mixture preparation and spectral collection.*