Evaluation of near infrared spectroscopy for assessing physical and chemical characteristics of linen weft yarn

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Introduction

Conventional chemical and physical methods of assessing yarn quality, although effective, are highly labour intensive. Within the linen industry there is a need for novel, rapid, non-destructive, instrumental means of predicting yarn quality. Current yarn production procedures are based on the blending of highly heterogeneous raw fibre supplies in order to enhance yarn consistency. Changes occurring in response to chemical processing, such as boiling, bleaching and dyeing can be detected and monitored by derivative thermogravimetry (DTG) and near infrared (NIR) spectroscopy. These methods allow sample homogeneity and quality parameters to be monitored during the various stages of processing.¹ Preliminary results suggest that NIR spectroscopy could also be useful during fabric finishing for assessing crease recovery and abrasion resistance performance.² The results from conventional physical and chemical analyses have provided supporting evidence for this. NIR spectra can be used to form predictive models allowing rapid assessment of yarn quality for physical and chemical characteristics.

Methodology

The yarn samples supplied for quality analysis were provided by Ferguson's Irish Linen (FIL), Banbridge, N. Ireland. All materials were sub-sampled (50 g) and conditioned for a minimum of 24 h at 20°C and 65% RH before analysis.

Derivative thermogravimetric analysis

Yarn samples were further sub-sampled (10 g) with representative material being cut to less than 1 mm length using a pair of serrated scissors. Thermogravimetric analysis using a robot (TSO 801 RO) controlled TGA/SDTA 851° (Mettler Toledo) instrument over a temperature range of 35–600°C at a 20°C rise min⁻¹ was carried out using 3.0–3.2 mg samples with a minimum of three replicates per treatment. The system was flushed with air at the rate of 20 ml min⁻¹ and the results analysed using Star (Mettler Toledo) software to calculate derivative peaks with their weight loss in the primary (220–400°C) and secondary decomposition (400–600°C) bands.

DTG thermograms, when overlaid, revealed that there was a high degree of similarity between individual sub-sample replicates. As DTG analysis can be performed on a variety of materials including raw fibre, roving and yarn, it may therefore be used to predict quality parameters.

Near infrared spectroscopy

Sub-samples of yarn were packed into closed cups comprising a quartz-glass cover and scanned ten times after re-packing with a Visual-NIR spectrophotometer (Foss NIRS 6500) at 2 nm intervals over the range 400–2498 nm producing 1050 data points. A band pass value of 10 nm was used with wavelength accuracy of \pm 0.5 nm. Reflectance readings were converted to absorbance (A) values using the equation: A = log (1/*R*). Infrasoft International software was used to collect the data and the raw spectral data exported for chemometric analysis (Unscrambler version 7.0, Camo, Trondheim, Norway).

Results and discussion

Derivative thermogravimetry

The most influential factor on yarn quality is processing sequence used during spinning. DTG analysis was performed on yarn samples supplied by three different spinners, the thermal profiles of which are presented in (Figure 1). Although maximum primary peak decomposition temperatures of the three test materials proved to be similar ($360-363^{\circ}$ C), primary peak weight loss of sample A was much higher (76.6%) than samples B (69.1%) and C (68.4%). Significant differences in terms of secondary peak weight loss, height and decomposition temperature were also observed. Peak two weight loss of Sample A was lower (16.4%) than B (24.1%) and C (25.73%), however, decomposition temperatures of B and C although similar (472° C), were much lower than sample A (492° C). The magnitude of the primary and secondary peak height and width parameters of yarn A compared to B and C would suggest that a greater quantity of non-cellulosic fractions were removed during the processing of A compared to the other two. This would infer that a more efficient processing treatment had been applied whilst spinning by the suppliers of this yarn. These distinct differences in yarn thermal profiles enable the prediction of valuable information on the process history of unknown yarn samples ³.

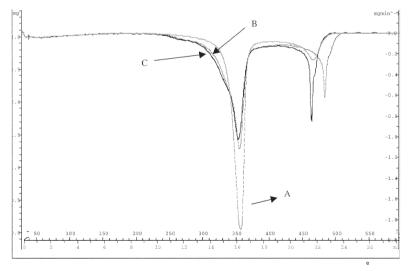


Figure 1. Overlay of 1st derivative thermograms of (a) good, (b) medium and (c) poor weft yarns.

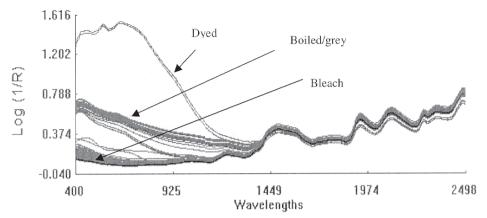
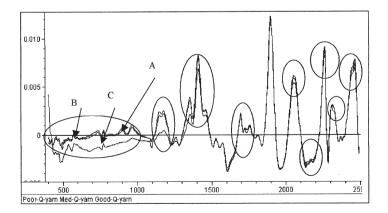


Figure 2. Raw NIR spectra indicating differences between boiled, bleached and dyed yarns.

Near infrared spectroscopy

Differences in yarn treatment and finishing processes have a direct effect on yarn performance characteristics such as tenacity and breaks during weaving. A variety of yarns that had been previously treated by alkali boiling, bleaching and dyeing were assessed using NIR. As shown in Figure 2, there were significant spectral differences between the three treated yarn types—both in the visible and near infrared wavelength bands. Bleached yarns have significantly lower reflectance values compared to dyed yarns in the visible spectral range. Within the near infrared regions the differences are much less clear and further manipulation of the raw spectra, for example by transformation, are necessary in order to highlight the variations.

In order to show how differences in key quality parameters are reflected by the spectral data, an extensive analysis of weft yarns using NIR spectroscopy was performed and a database of yarns with different known quality characteristics developed. Three grades of weft yarn were assessed using NIR



| Parameters | n | SEC | R^2 | SECV | R^2 |
|------------------------------|----|--------|-------|--------|-------|
| Tenacity cN/Tex | 46 | 0.01 | 0.98 | 1.21 | 0.75 |
| CV-Mass (%) | 48 | 1.11 | 0.78 | 1.41 | 0.62 |
| Neps 200/km | 45 | 293.60 | 0.94 | 505.50 | 0.81 |
| Elongation (%) | 46 | 0.09 | 0.89 | 0.01 | 0.71 |
| Degree of polymerisation | 47 | 348.30 | 0.84 | 471.24 | 0.70 |
| Cautic weight loss (CWL) (%) | 50 | 2.19 | 0.89 | 2.99 | 0.78 |
| Calcium (ppm) | 40 | 545.00 | 0.86 | 678.60 | 0.78 |
| Nitrogen (%) | 32 | 0.01 | 0.98 | 0.001 | 0.96 |
| Carbon (%) | 48 | 0.36 | 0.90 | 0.464 | 0.83 |
| Ash (%) | 36 | 0.13 | 0.85 | 0.72 | 0.17 |

Table 1. Preliminary NIR calibrations for the assessment of weft yarn quality.

SEC: standard error of calibration

SECV: standard error of cross-validation

spectroscopy. The raw spectral data were transformed and the spectra presented in Figure 3. The greatest variation in yarn type was observed in the visible spectral region due to different bleaching treatments used, however additional differences were also observed in the 1100–1200, 1300–1400, 2060, 2146–220, 2312 and 2450 nm wavelengths. Partial least squares calibrations for key physical properties, such as tenacity, CV-mass, neps and elongation, and chemical characteristics, such as degree of polymerisation, caustic weight loss, calcium, nitrogen, carbon and ash, of weft yarn have been developed using the visible and NIR spectra (Table 1). However, r^2 values for both calibration and cross-validation of the parameters need to be improved with additional sample sets. The results have shown that spectroscopy has the potential for assessing yarn quality rapidly.

Conclusion

Quality assessment system using spectroscopy to monitor key yarn parameters is feasible and hence enhancing yarn and fabric quality optimisation during production is possible, provided robust predictive models can be developed. Such a system, supported by additional DTG analysis, would enable rapid, accurate prediction of yarn performance during all stages of processing and thus reducing problems arising from variation in raw material quality.

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