

## Quantification of components of textile fabrics by using chemometric techniques with FT-NIR spectroscopic data

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### Abstract

The study has attempted to develop chemometric modeling based method to quantify compositions of textile fabrics by FT-NIR spectroscopic data. Three calibration techniques such as: Principal Component Regression (PCR), Partial Least Square Regression (PLSR) and Artificial Neural Network (ANN) were assessed, and PLSR showed the best result. Several pretreatment techniques of spectral data have been evaluated, and Multiplicative Scatter Correction (MSC) performed the best. Results also shows that performance of PLSR was satisfactory for quantification of cotton ( $R^2 \approx 0.99$ ), elastine ( $R^2 \approx 0.97$ ) and polyester ( $R^2 \approx 0.94$ ) when FT-NIR spectral data were pretreated with MSC. But for quantification of viscose in mixture fabric, efficiency of developed model was not upto the mark ( $R^2 \approx 0.75$ ). Finally, the developed PLSR model with FT-NIR spectroscopic data pretreated with MSC could be used for quantification of cotton, elastine and polyester in textile fabrics rapidly and with comparatively low cost.

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### Introduction

One of the key sectors of rapid growing economy of Bangladesh is manufacturing and exporting textile and clothing products (Akhtaruzzaman, 2018). Exports of textiles and garments are the principal source of foreign exchange earnings in the country. It also provides employment to around 4.2 million Bangladeshis, mainly women from low income families (Hasan *et al.* 2016). Garment fabrics are unifabric cotton (100%), viscose (100%), polyester (100%), etc. or mixture of these components usually in different proportions. Therefore, textile products must be marked with fabric type and composition on the label as per demand of buyers to maintain the quality of the products. So, assessment of the compositions in fabric is an essential part for maintaining the quality of the garment products.

Traditional methods have been used to identify different fabric classes, their properties, and their morphological differences normally require extensive testing and

complicated time-consuming analysis. These methods, which are based on physical, chemical, and microscopic techniques, are somewhat limiting, since successful identification depends upon experience and familiarity with the fabrics.

For determining properties of textile fabrics (Stankovic *et al.* 2008; Romeli *et al.* 2013), knitted fabrics (Majumdar *et al.* 2010), and recycled textile fabrics (Hadded *et al.* 2016) different methods have been used.

Vibrational spectroscopic technique, an alternative approach, which is generally quicker and more robust, can be used. Multivariate or chemometric analysis of Ultraviolet (UV), Near-infrared (NIR) and other spectroscopic data have become a novel qualitative and quantitative analysis technology and are widely applied in several fields including the food (Uddin *et al.* 2017),

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Pharmaceutical (Israt *et al.* 2016), pulp and paper (Uddin *et al.* 2019a; Uddin *et al.* 2019b) and petrochemical (Hossain *et al.* 2018) industries for nondestructive, simple, and fast process and nearly require no sample pretreatment. Moreover, spectroscopy is a useful qualitative method to characterize raw materials and finished textile products. The chemometric methods with spectroscopic data provide approach to quantify key chemical, physical and morphological properties of textile fibers, yarns, fabrics, and chemical textile auxiliaries rapidly, accurately and precisely.

The use of spectroscopic data with chemometric modeling in the textile industry is comparatively new. Soft independent modeling of class analogy (SIMCA) has been used for classification or identification of textile fabrics with NIR (Cleve *et al.* 2000; Busch *et al.* 2012; Davis *et al.* 2015) and discriminate analysis based on Principal Component Analysis (PCA) ATR-FT-IR (Peets *et al.* 2017) data. In 2016, a group of scientists from China developed a similar method for classification of textile fabrics (Cotton, Viscose, Acrylic, Polyamide, Polyester and Blend) with Pattern Recognition Method (Sun *et al.* 2016) for quantification of compositions in textile fabrics. Some other studies have been reported where chemometric techniques were used with spectroscopic data for classification of textile fabrics (Durand *et al.* 2007).

Chemometric models were developed by Ruckebusch *et al.* (2006) with FT-NIR spectroscopic data for quantitative determination of cotton, and by Chen *et al.* (2020) with NIR spectroscopic data for quantification of wool, polyester, polyacrylonitrile, and nylon in textile blends.

However, no research work has been reported to develop method for quantification of viscose and elastine in textile fabrics with chemometric modeling of preprocessed FT-NIR spectroscopic data. Therefore, the present study has attempted to develop a method for quantification of cotton, viscose, polyester and elastine in textile fabrics by chemometric calibration techniques with FT-NIR spectroscopic data where the spectroscopic data were pretreated or preprocessed with several transformation techniques.

## Materials and methods

### *Samples*

Total 90 samples were collected from 5 different garments manufacturing factories of the Bangladesh Small and Cottage

Industries Corporation (BSCIC) in industrial area in Narayangong district of Bangladesh. The fabrics are of 100% cotton (20), 100% Elastine (10), 100% polyester (10), and blend of cotton and others in different proportions (50). Garments factories get the tested results from TUV, SUB Bangladesh Ltd. (a testing and certification regulator), They preserve these data with respective samples for their buying compliances, and for further reference. In the study, those tested results of fabric compositions have been used with FT-NIR spectroscopic data for model development.

### *Spectral data collection*

Chemical properties are specific chemical species or groups present in the material (i.e. CH, OH, NH) that result in FT-NIR spectral absorbencies at distinctive wavelengths. Fourier Transformed Near Infrared Spectroscopy (FT-NIR) spectroscopy was performed using a PerkinElmer FT-IR/NIR spectrometer (Model: Frontier, Perkin Elmer, USA) with GAAS detector. The spectral range used was 12,000-4,000 $\text{cm}^{-1}$ . For each sample, 32, scans were collected at a spectral resolution of 16 $\text{cm}^{-1}$  with an interval of 4  $\text{cm}^{-1}$ , then the 32 scans were averaged and stored as reflectance percentage (%R). Here PerkinElmer Spectrum (Version 10.4.4) software was used for spectral data processing.

### *Preprocessing of spectral data*

After acquisition of spectral data from FT-NIR, at first they were preprocessed with some transformations. In the study, three smoothing techniques such as Savitzky-Golay (S-G) smoothing, Mean Normalization, Standard Normal Variate (SNV) and Multiplicative Scatter Correction (MSC) were applied and their efficiencies were assessed. Among them, MSC showed incomparably better results than others. Therefore, results shown here are based on the data pretreated with MSC.

### *Multiplicative Scatter Correction (MSC)*

MSC is a scatter correction method which is based on the idea of correcting the scatter level of all spectra of a group of samples to the level of an "ideal" sample's spectrum, which is usually the average spectrum (Geladi, 2003). This is possible because light scatter's wavelength dependency is different from that of chemically based light absorption. MSC is a set dependent transformation. If the raw data set is modified, the ideal spectrum, i.e. the mean spectrum, is likely to be improved for better predictive modeling.

### *Principal Component Analysis (PCA)*

PCA is the most frequently used tool in Chemometrics to reduce dimensionality of data and many other reasons through latent variables, Principal Components (PCs) (Jolliffe, 2002). The main purpose of PCA is to reduce the dimensionality of a data set consisting of a large number of interrelated variables to a much smaller number, while retaining as much as possible of variation present in the data set (maximum variance). The PCs are uncorrelated and ordered so that the first few retain most of the variation present in all of the original variables. Thereby, the measured variables (absorbance at different wavelengths) are converted into new variables called scores.

### *Calibration model development*

Predictive efficiency of calibration techniques such as PCR, PLSR and ANN have been assessed for quantification of constituents of textile fabrics with FT-NIR spectral data.

### *Principal Components Regression (PCR)*

PCR is a procedure for analyzing multiple regression when the data are multicollinear. It is a two-step multivariate calibration technique. Initially, a Principal Component Analysis (PCA) of the spectral data matrix is done. Absorbance at different wavelengths are transformed into new scores on dormant variables. Next step is a multiple linear regression (MLR) between the scores found in the PCA step and the known composition of mixed textile fabrics (Jolliffe, 2002).

### *Partial Least Square Regression (PLSR)*

PLSR finds components from independent variables (X) that best predict the dependent variable (Y). To be specific, PLSR looks for a set of components (latent variables) that accomplishes a simultaneous decomposition of X and Y with the restraint that these components elucidate as much as possible of the covariance between X and Y. PCA are created in this step. Next, is a regression step where the latent variables gained from X are used to forecast Y. PLSR decomposes both X and Y as a product of a common set of orthogonal factors and a set of certain loadings (Wold *et al.* 2001).

### *Artificial neural network (ANN)*

ANN is a multivariate procedure that is like human brain and nervous system in learning from experience. ANN are more commanding than traditional approaches in situations when the problem require qualitative or complex quantitative reasoning where the conventional statistical and mathematical methods are poor or the parameters are highly independent and data are inherently noisy, imperfect or error prone. ANN is an interconnected group of nodes, akin to the vast network of neurons in the human brain. It is a data processing system grounded on the construction of the biological neural simulation by learning from the data produced from an experiment or by using authenticated models (Bishop, 1995). Here, Levenberg-Marquardt back-propagation artificial neural network has been used. Ten hidden neurons and the sigmoid activation function have been used here in each training as they have produced better predictive results than other alternatives.

### *Cross-validation*

To evaluate the efficiency of the developed model, six fold cross-validation techniques has been used in all cases. These process will help to minimize the threats of over-fitting of the constructed models.

### *Software for model development*

For calibration and validation of PCR and PLSR and a software, CAMO the Unscrambler of its version 10.3, was used, and for ANN, the Matlab (version 2016a) was used in this study.

## **Results and discussion**

In the mixed samples, the components are cotton, elastine, viscose and polyester and they are blended in different proportions. The descriptive statistics of proportions of these components are presented in table I.

**Table I. Descriptive statistics of proportions of components in mixed samples**

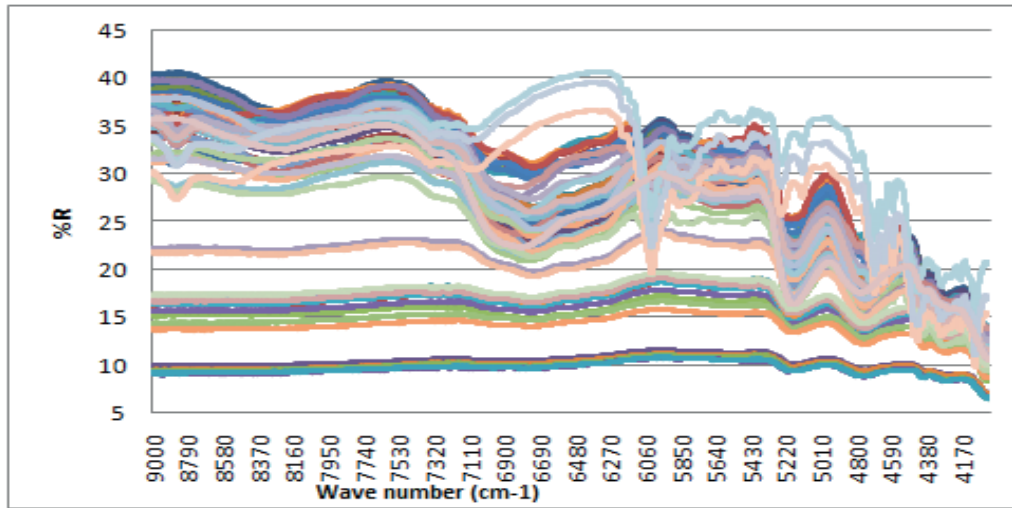
Components	Minimum (%)	Maximum (%)	Mean (%)	Standard deviation
Cotton	0	98.00	71.07	28.86
Elastine	0	5.00	0.84	1.67
Viscose	0	97.00	8.59	17.12
Polyester	0	65.00	17.49	24.39

Major component in the mixed fabric samples is cotton with is upto 98% with an average of 71.07% and standard deviation (SD) 28.86. Polyester is another pivotal component in these mixtures which is up to 65% with an average 17.49% and SD 24.39. There are some samples which have viscose and Elastine consisting of 8.59% and 0.84% respectively.

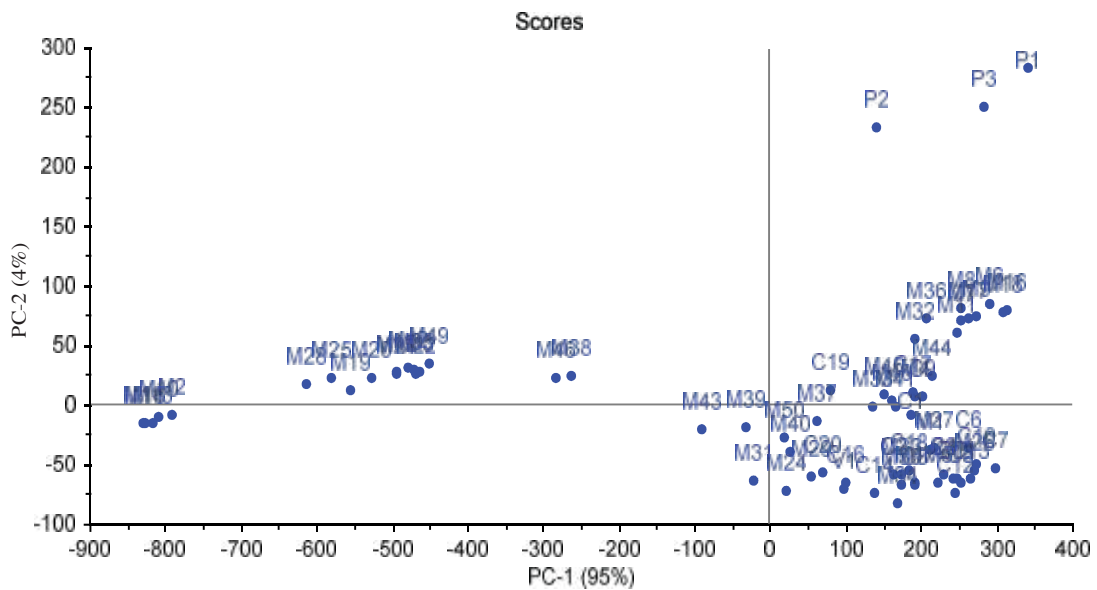
Spectroscopic data of 90 textile fabric samples for FT-NIR data are plotted in figure 1.

*Principal component analysis*

From the Principal Component Analysis (PCA) of the FT-NIR spectroscopic data, the first principal component (PC1) express 95% of the variation whereas PC2 express 4% of the total variation. Therefore, the total 99% is sufficiently good for developing multivariate analysis based chemometric models with spectroscopic data.



**Fig. 1.** Combined presentation of FT-NIR spectral data



**Fig. 2.** Score plot

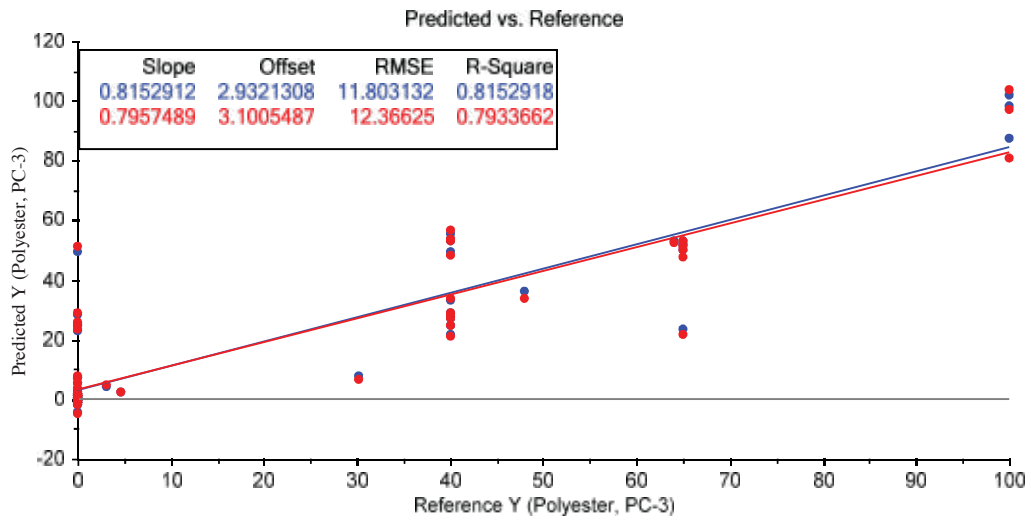


Fig. 3. PCR model for quantification of polyester with raw data

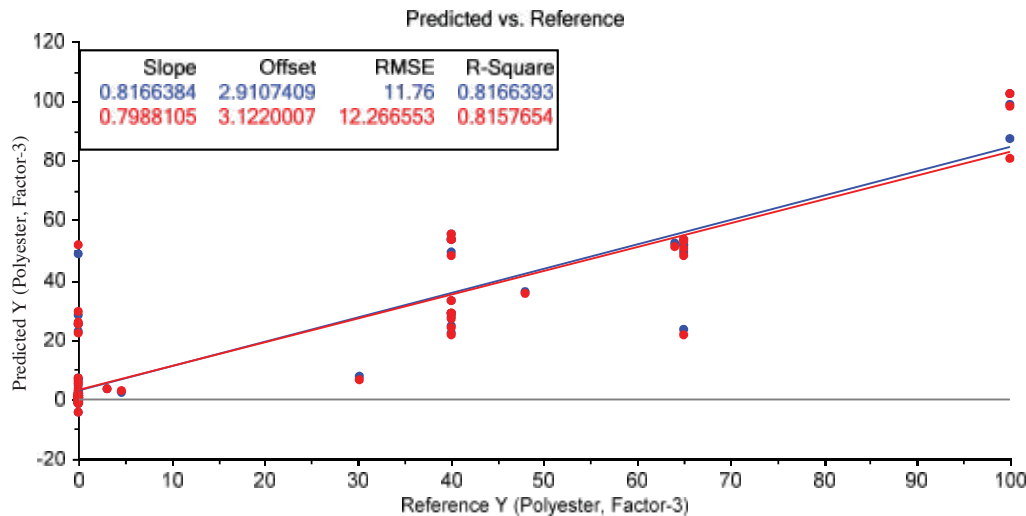


Fig. 4. PLSR model for quantification of polyester with raw data

The score plot, also called map of samples, shows that the samples are scatterly distributed without following any pattern which is an indication of appropriateness of the data for modeling.

*Principal component regression (PCR)*

Model parameters namely slope and offset are 0.815 and 2.932 respectively in the PCR model presented in the figure 3. This PCR model has been developed with raw FT-NIR spectroscopic data for prediction of Polyester in mixed textile fabrics.

To assess the predictive efficiency of model, Root Mean Square Error (RMSE) and coefficient of multiple determination ( $R^2$ ) as model efficiency parameter were used in this study. RMSE and  $R^2$  are 11.80 and 81.23% for calibration dataset, and 12.37 and 79.34% for validation dataset respectively.

Model parameters (Slope and Offset) and model efficiency parameters (RMSE and  $R^2$ ) along with plotted points are in blue colors for calibration dataset and in red colors for cross-validation datasets. Parameters for both calibration and

validation datasets are very close which means that the developed PCR model is stable and there is to problem of over-fitting. The model has been developed with first three latent variables (LVs), or components as it produces the best results.

*Partial least square regression (PLSR)*

Another multivariate calibration technique, Partial Least Square Regression (PLSR) is also assessed for quantification of compositions in mixed textile samples.

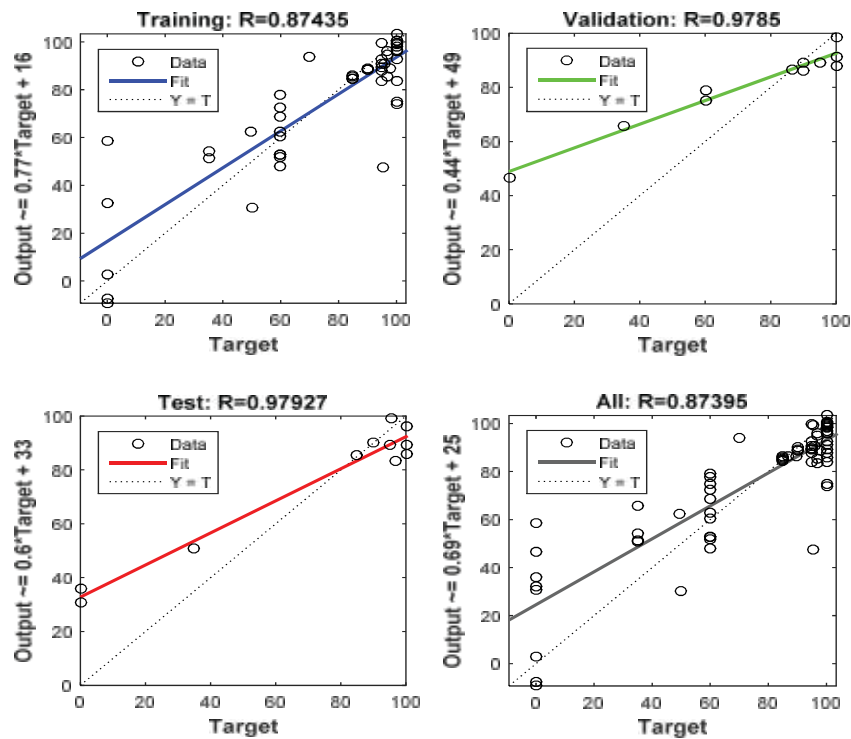


Fig. 5. ANN model for quantification of cotton with raw data

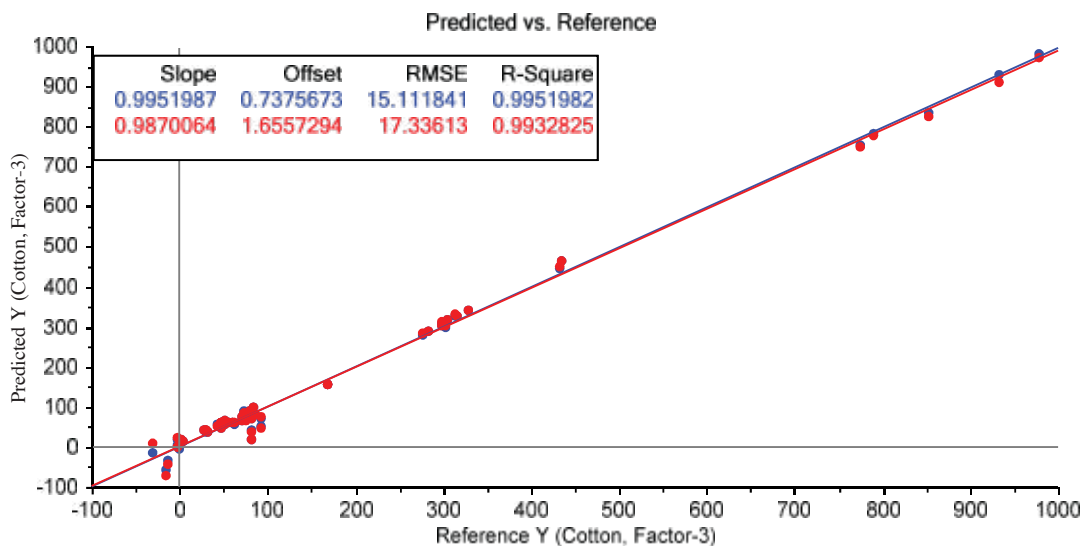


Fig. 6. PLSR model for quantification of cotton with MSC pretreated data



The results from PLSR model is as good as those of PCR with raw spectroscopic data for prediction of polyester in mixed textile samples ( $R^2 \approx 82\%$ ) both for calibration and cross-validation datasets. The model is a stable one with high validation dataset ( $R^2 \approx 82\%$ ). Here first 3 latent variables (factors) have been used to construct the model as it produces the best results.

*Artificial neural network*

Artificial Neural Network (ANN) is comparatively new calibration technique. It is getting popularity in chemometric analysis, and have rarely used in textile fabric analysis. ANN shows relatively better results for prediction of cotton and polyester with raw spectroscopic data ( $R^2 \approx 82\%$ ). But for

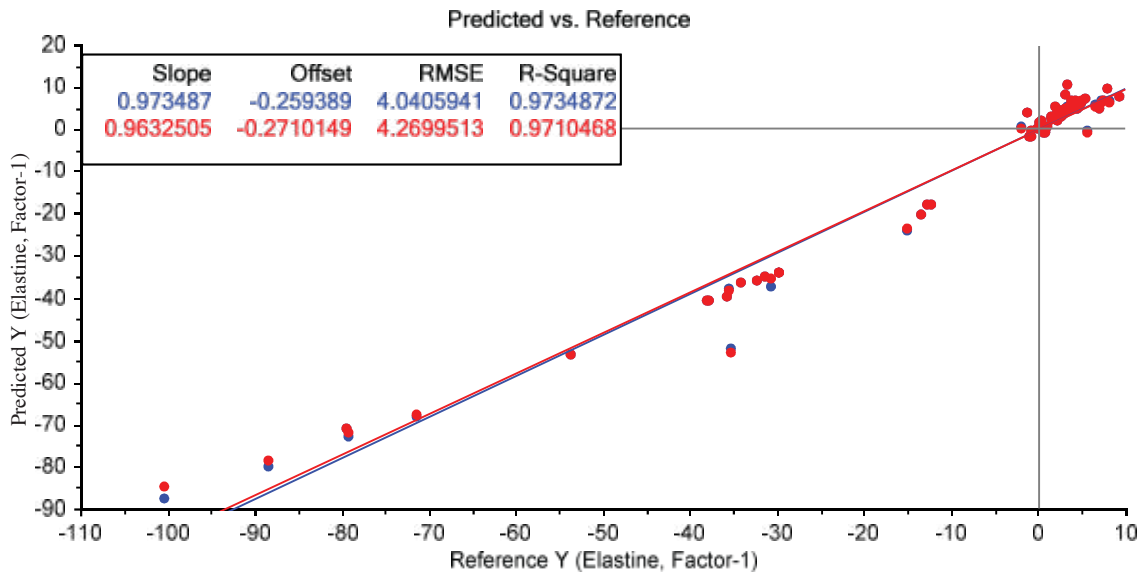


Fig. 7. PLSR model for quantification of elastine with MSC pretreated data

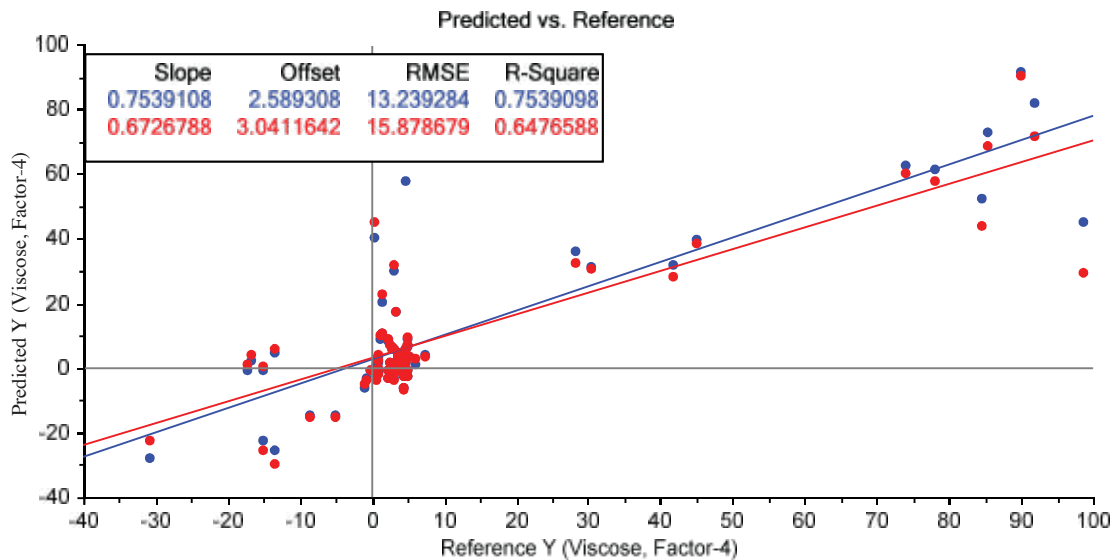


Fig. 8. PLSR model for quantification of viscose with MSC pretreated data

elastine and viscose, performance of this calibration technique is not satisfactory as respective  $R^2$  are 15% and 53% only.

Among PCR, PLSR and ANN, Partial Least Square Regression (PLSR) showed consistently the best results for quantification of cotton, elastine, viscose and polyester in mixed textile fabrics. Therefore, in quest of the best models

PLSR model for cotton,  $R^2$  is more than 99% both for calibration and validation datasets. It requires only 3 factors to construct the model. It is a very stable model to be used in practical situation as both the calibration and validation  $R^2$ 's are very high.

For quantification of elastine, the results are also satisfactory ( $R^2 \approx 97\%$ ) with MSC treated spectroscopic

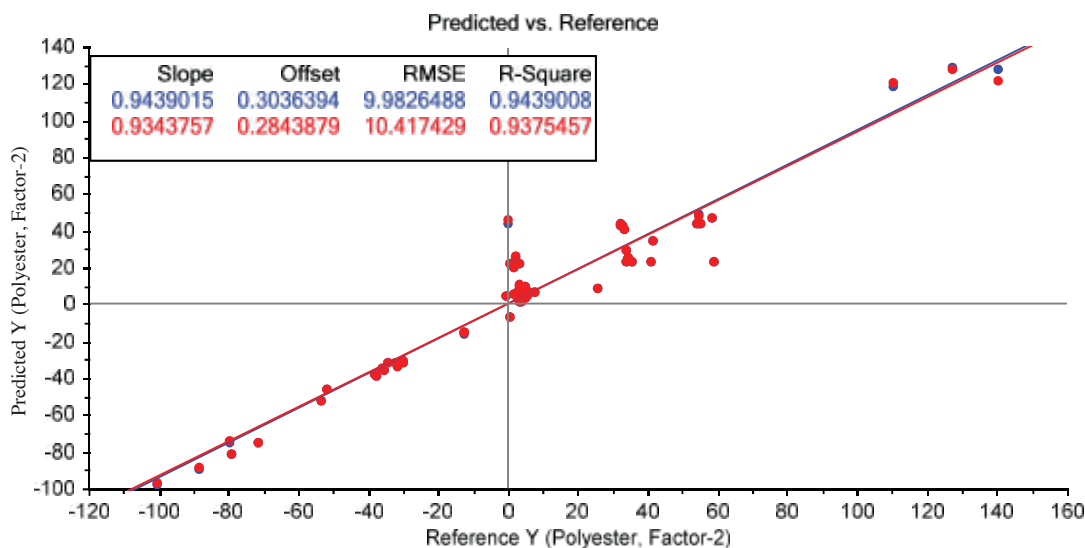


Fig. 9. PLSR model for quantification of polyester with MSC pretreated data

for prediction of these elements in the textile samples, PLSR has been chosen.

#### Modeling with preprocessed spectral data

The efficiency of the models with raw spectroscopic data are not satisfactory to be used for the predictive purpose for quantification of compositions in mixed textile fabrics. Some treatments as a part of preprocessing of FT-NIR spectroscopic data could be one of the solutions. Therefore, the spectroscopic data were preprocessed with several pretreatment techniques like Savitzky-Golay (S-G) filtering, Mean Normalization, Standard Normal Variate (SNV) and Multiplicative Scatter Correction (MSC).

None of the techniques except MSC, showed good result for prediction of all compositions in the mixed samples. So, efficiency of PLSR were assessed for quantification of constituents in textile fabrics with pretreated data with MSC.

After pretreatment of spectral data with MSC, PLSR model showed very good predictive performance for quantification of each constituents in fabrics. Here, in

data both for calibration and validation datasets, and the model was constructed with only the first latent variable.

Predictive efficiency of PLSR model in terms coefficient of multiple determination is not satisfactory ( $R^2 \approx 75\%$ ) for quantification of viscose with MSC pretreated data. The model is bit unstable as well. The model requires 4 factors to reach to its best performing results.

In case of predicting Polyester, PLSR model produce very good results ( $R^2 \approx 94\%$ ) with MSC treated spectroscopic data. The model is stable enough as the results for calibration and validation datasets are very close, and the model needs only 2 factors.

For quantification of Cotton, Elastine, Viscose and Polyester in mixture textile fabrics, three multivariate calibration techniques namely Principal Component Regression (PCR), Partial Least Square Regression (PLSR) and Artificial Neural Network (ANN) have been used both with raw FT-NIR data and pretreated data with Multiplicative Scatter Correction (MSC). The results from these techniques did not produce satisfactory results with raw spectroscopic data. So,



**Table II. Comparison among predictive models**

Fabric composition	Dataset	Raw data				Treated with MSC			
		PCR		PLSR		ANN		PLSR	
		RMSE	R <sup>2</sup>	RMSE	R <sup>2</sup>	RMSE	R <sup>2</sup>	RMSE	R <sup>2</sup>
Cotton	Calibration	15.70	0.76	15.50	0.77	14.07	0.82	15.11	0.995
	Cross-validation	17.84	0.68	18.46	0.68			17.34	0.993
Elastine	Calibration	1.35	0.08	0.98	0.52	1.12	0.15	4.04	0.973
	Cross-validation	1.39	0.05	1.25	0.24			4.27	0.971
Viscose	Calibration	12.38	0.53	12.56	0.52	13.34	0.53	13.24	0.754
	Cross-validation	14.88	0.29	15.24	0.29			15.88	0.648
Polyester	Calibration	11.80	0.82	11.76	0.82	12.85	0.82	9.98	0.944
	Cross-validation	12.37	0.79	12.27	0.82			10.42	0.938

pretreatment of these data was required. After applying different pretreatment techniques like 1<sup>st</sup> and 2<sup>nd</sup> derivatives, Smoothing and Savitzky-Golay (S-G) filtering and Multiplicative Scatter Correction (MSC), MSC showed the best results with PLSR. R<sup>2</sup> is very high (R<sup>2</sup>=94-99%) for predicting all parameters except for viscosity (R<sup>2</sup>≈75%). The predictive performance of these models are very stable as the results with calibration and cross-validation datasets are very close and very high (R<sup>2</sup>=94-99%). The results for cotton are very similar to those of Durand *et al.* (2007). The models for quantification of polyester and elastine in mixed textile fabrics by chemometric calibration techniques are novel, and no study has been reported yet.

### Conclusion

In this study, a cost effective and simple method has been developed for rapid quantification of textile fabric compositions by FT-NIR spectroscopic data and chemometric calibration techniques. Results shows that PLSR produced consistently better results than PCR and ANN. Result of the models are not satisfactory with raw spectroscopic data and therefore, some transformation of the data were required. Here, MSC shows the best results. Finally, the predictive performance of PLSR with pretreated FT-NIR data with Multiplicative Scatter Correction (MSC) is satisfactory for cotton (R<sup>2</sup>≈0.99), elastine (R<sup>2</sup>≈0.97) and polyester (R<sup>2</sup>≈0.94). But for quantification of viscose in mixture fabric is not upto the mark (R<sup>2</sup>≈0.75).

By using the developed models with treated FT-NIR Spectroscopic data by MSC, garments factories and related testing laboratories could quantify the percentage of cotton, elastine and polyester in mixed textile fabrics easily and efficiently. This method is a green, non-destructive, rapid and simple to use for garments manufacturing industries and relevant testing laboratories.

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