Proceedings of the 51st International Convention of Society of Wood Science and Technology
November 10-12, 2008 Concepción, CHILE

Prediction of Yellow-Poplar (*Liriodendron tulipifera*) Veneer Stiffness and Bulk Density Using Near Infrared Spectroscopy and Multivariate Calibration

Oluwatosin E. Adedipe
Ben Dawson-Andoh
Division of Forestry and Natural Resources, Davis College of Agriculture, Forestry, and Consumer Sciences, West Virginia University, Morgantown, WV. 26506-6125. USA.
Email: oadedipe@mix.wvu.edu, bdawsona@wvu.edu

Abstract

This study investigated the feasibility of using near infrared (NIR) spectroscopy and multivariate calibration to predict stiffness and bulk density of 3.2 mm thick Yellow-Poplar veneer strips. Full-range (800-2500 nm) raw NIR spectra and spectra pre-treated using the first derivative method, along with spectra from three other different wavelength windows of 1200-2400 nm, 1800-2400 nm and 1400-2000 nm were regressed against the dynamic modulus of elasticity (stiffness; GPa) and the bulk density (kg/m^3) values of the veneers using the projection to latent structures (PLS) method to develop calibration models. All predictive models developed performed well in the prediction of stiffness and bulk density of new test samples that were not included in the calibration models. R^2 values ranged from 0.56- 0.72 and 0.67-0.78 respectively for stiffness and bulk density. There was significant improvement in models developed with first derivative spectra over models developed with raw spectra. The models developed using the first derivative used fewer latent variables to achieve predictive models with higher R^2 values, lower root mean square errors of prediction (RMSEP) and standard errors of prediction (SEP). Models developed using the full NIR spectra range (800-2500 nm) and the NIR spectra region of 1200 -2400 nm performed better than models developed using the restricted NIR wavelength regions of 1800-2400 nm and 1400-2000 nm. However, there was no clear distinction between models developed using the full NIR spectra range and the NIR spectra region of 1200-2400 nm. Overall, models developed with the first derivative pre-processed spectra using the whole NIR spectra performed best in predictability. The results of this study show the potential of using multivariate data analysis coupled NIR spectroscopy for on-line sorting and assessment of veneer stiffness prior to the lay-up process in the manufacturing of veneer-based engineered wood products such as plywood, Parallam and laminated veneer lumber.

Keywords: Near infrared spectroscopy, veneer, dynamic modulus of elasticity, bulk density, Yellow-Poplar, multivariate data analysis, partial least squares regression.

Introduction

The manufacturing process of plywood, Oriented Strand Board (OSB), Laminated Veneer Lumber panel (LVL) and Parallam involves gluing of individual veneer sheets, strips or strands to form panels. Therefore, it will be of great benefit to these industries if the main raw material could be sorted on the basis of stiffness strength prior to the lay-up of the panels. This study is a follow up to the previous study (Meder *et al.* 2000), as we attempt to use a dynamic measure of stiffness as the NIR-predicted variable. It also addresses the issue of measuring veneer stiffness via a direct measure as this is desirable in a mill environment. This will enable the production of "designer" engineered wood products, more consistent product; reduce waste, improve the use of raw material resources and reduce the cost of the manufacturing process.

Objective of study

The aim of this study was to examine the possibility of using NIR spectroscopy to predict the stiffness strength of veneer strips and sort veneer strips based on bulk density. If feasible, subsequent studies could then evaluate its application in a mill environment.

.

Materials and methods

Veneer specimens of yellow-poplar (*Liriodendron tulipifera*) veneer strips used for this study were provided by Truss Joist, A Weyerhaeuser Business, Buckhannon, WV, USA. The veneer specimens had been previously processed in the plant into strips, as used in the manufacture of LVL and Parallam panels from rotary-peeled 3.2 mm nominal thickness yellow-poplar veneer sheets. The yellow-poplar veneer strips were of two different colors (clear yellow and greenish brown) and they included all random defects such as cracks associated with structural veneer used in engineered veneer-based wood products. A total of 400 samples were used for the study. All the 400 samples were cut to a length of 190 mm, while the width and thickness was determined at the factory. The average dimensions for the veneer strips were 190 mm x 16 mm x 3.2 mm. The veneers were oven-dried at 103±2 ^{0}C for 24 hours to a moisture content of approximately 3% in order to maintain uniformity and reduce error due to variation in moisture content of the samples.

All the veneer strips were weighed on an analytical balance to determine the mass of individual veneer strip, and later measured along the length, width and thickness using a digital caliper (Fisher Scientific, Pittsburgh, PA, USA) to determine the exact dimensions. The bulk density of each veneer strip was calculated as a ratio of mass (kg) : volume (m^3).

Dynamic modulus of elasticity (MOE) was determined using longitudinal (ultrasonic stress wave) resonance measuring equipment. The two sides of the veneer strips were measured because it was difficult to determine the tight or loose side from the veneer specimens that had been processed in the plant into strips. The average of the propagation time of the two side of each specimen was used in calculating the dynamic MOE. The longitudinal stress wave was measured using an ultrasonic timer with two special

triangle-shaped piezoelectric accelerometers attached with a cylindrical part (FAKOPP Microsecond Timer; FAKOPP Enterprise, Agfglva, Hungary;" Figure 1").

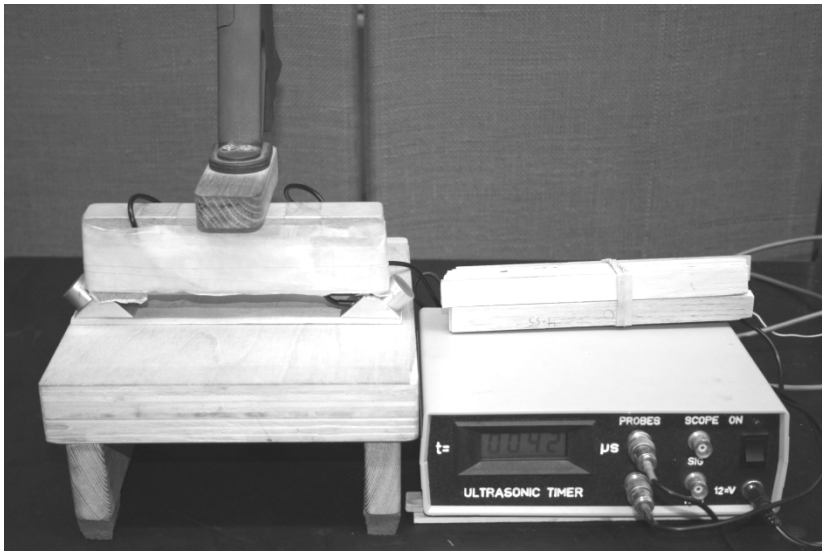

Figure 1. Fakkop ultrasonic timer and 45 KHz piezo electric transducers

The transducers used a 127 V, 45 kHz impulse that lasted for 30 seconds. The subsequent impulses were generated at one second intervals. Sand paper was used as a coupling material to generate a surface pressure of 3-4 MPa between the transducers and veneer sheets. The propagation velocity of longitudinal stress waves in a material are directly related to the modulus of elasticity and the bulk density of the substance, and hence the dynamic modulus of elasticity (E_d) is calculated as:

$$E_d = \acute{\upsilon}^2 \rho \qquad \text{"Equation (1)"}$$

Where:

E_d ----- dynamic Modulus of Elasticity (Pa)
ύ- ------propagation velocity (m s^{-1})
ρ -------density (kg m^{-3})

The NIR spectrum of each sample was collected with an FT-NIR spectrometer (Matrix-F; Brüker, Billerica, MA, USA) fitted with a fiber optic sampling probe for solids and operating in a diffuse reflectance mode with approximately wavelength range of 800 nm to 2500 nm. Each specimen was scanned at both side, twenty times per spot at two spots on the opposite ends of the veneer strips. The twenty scanned spectra per spot were averaged into one spectrum; overall there were four spectra per specimen (two spectra per side).

Development of NIR calibration

All the average spectral data obtained from the 400 yellow-poplar samples were used for the study. They were divided into calibration and prediction sample sets. The calibration

data set (n=200) consisted of all the odd numbered spectra between 1 and 400, while the validation set (n=200) comprised all even numbered samples. Calibration models were developed using the raw spectra and spectra pre-processed using the Savitsky-Golay first derivative order. The calibration spectra data were used in computing the partial least squares regression (PLS). All the NIR spectra were combined into a single data matrix (X-matrix) while the bulk density values and E_d values were combined into a separate Y1-matrix and Y2- response matrix respectively. Separate calibration models were developed for four different NIR spectral regions. The calibration models were constructed with 190 spectral samples, after removing ten outlier spectral samples, using full cross- validation method. Ten spectral samples were removed because the score plot of the PCA analysis showed them to be separate from the rest of the samples to a larger extent. This fully cross-validated model was then used to predict the response of the prediction set (test set) that comprised 200 samples that were not included in the original calibration model.

Results and Discussion

The bulk density of the veneer strips ranged from 321-576 kg/m^3 while the E_d values for the veneer strips ranged from 5.07-9.58 GPa. "Figure 2" shows plots of the full NIR (800-2500 nm) raw spectra used to develop calibration models. All the spectra looked very much alike, and it was difficult to see any spectral pattern because the maxima peaks in the NIR spectral region of 1400-2200 nm showed broad humps. "Figure 3" shows the plots of full NIR spectra (800-2500 nm) pre-processed using the 1st derivative method with distinct maximal and minimal peaks in the NIR spectral regions of 1300-1500 nm and 1700- 2200 nm respectively.

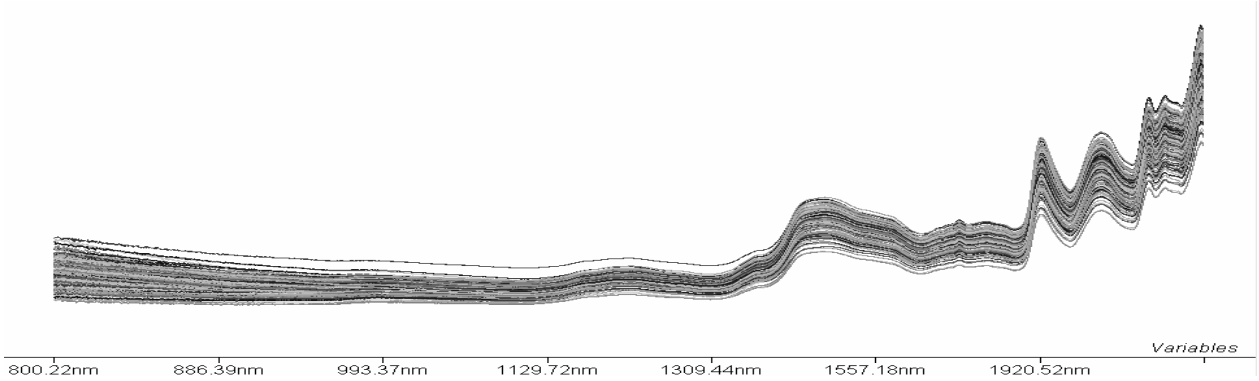

Figure 2. Representative raw spectra of yellow poplar veneer

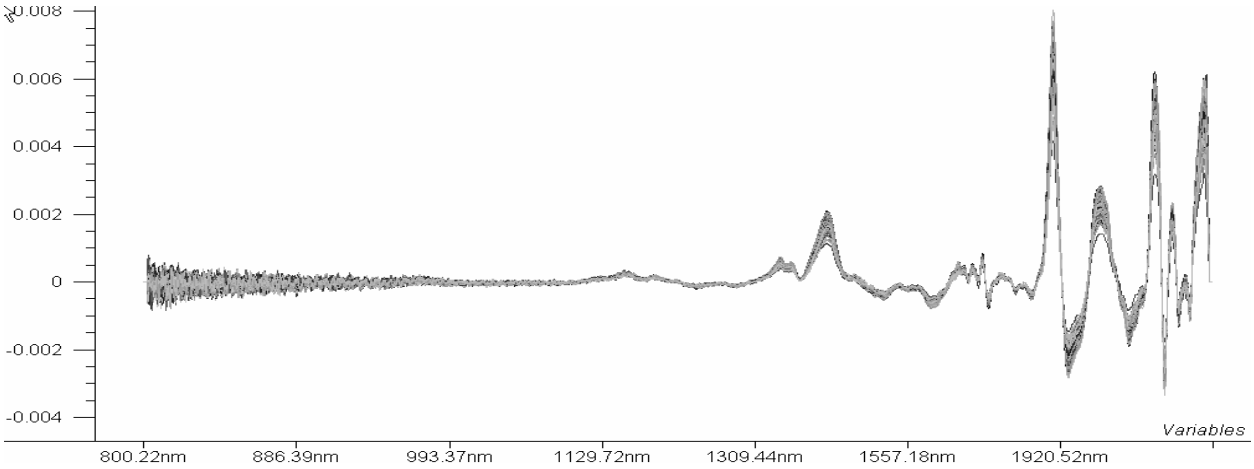

Figure 3: Spectra of yellow poplar veneer after pre-processing with first derivative transformation

Clustering of veneer samples was observed when a preliminary principal component analysis (PCA) with no Y-response values was carried out on the raw spectral data and data pre-treated using the 1st derivative method as shown in "Figure 4". The clustering observed in the score plot of the PCA may be attributed to the variation in the sample population as a result of the color variation of the yellow- poplar sample. There was no distinct clustering of samples when the partial least squares regression (PLS) was carried out using the density and Ed values respectively as the Y values. "Figure 5" shows the score plots for the PLS analysis with the density (kg m^{-3}) as the Y-response value.

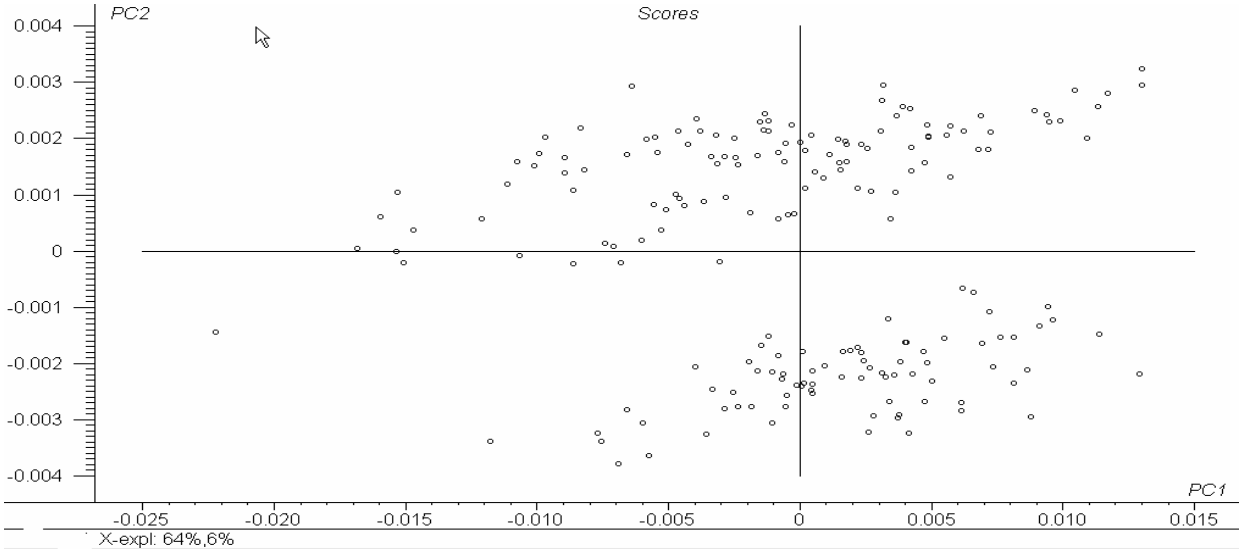

Figure 4: Score plot of the principal component analysis (PCA) of full NIR spectra (800-2500 nm) pre-treated with first derivative transformation method showing clustering of veneer samples

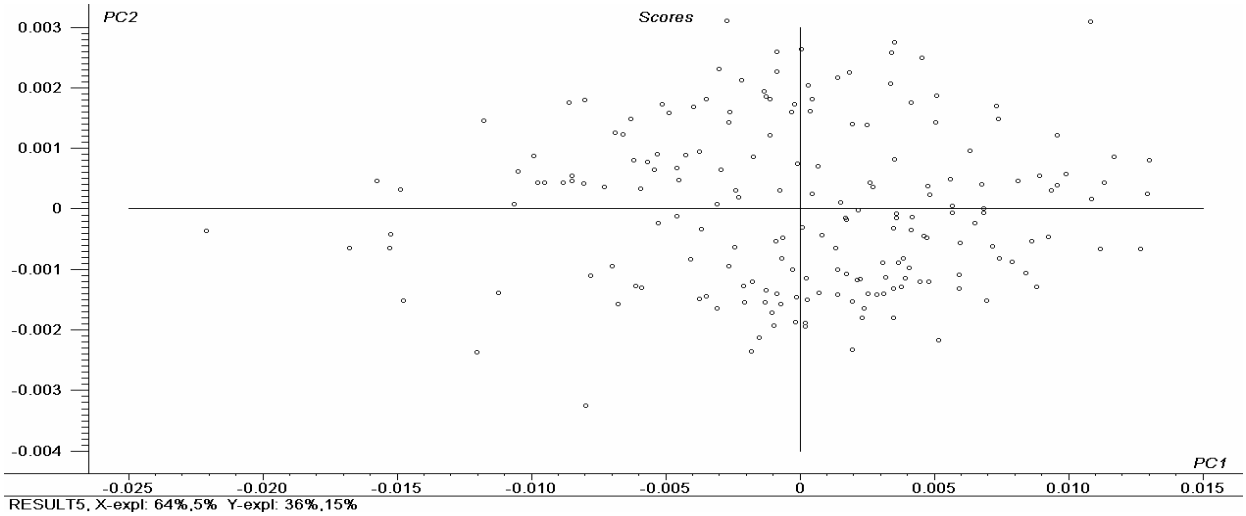

Figure 5: Score plot of the partial least squares regression (PLS) of full NIR spectra (800-2500 nm) pre-treated with first derivative transformation method showing clustering of veneer samples.

"Table 1" shows the result of models developed for the four NIR spectral regions for the prediction of density (kg/m^3) using raw spectra and the spectra pre-processed using the 1st derivative method, while "Table 2" shows the result of models developed from the four NIR spectral regions for prediction of E_d (GPa) using raw spectra and for spectra pre-treated using the 1st derivative method. The performance of the PLS models developed for this study were evaluated using the correlation coefficient of determination (R^2) between predicted and measured values, the standard error of calibration/ prediction (SEC/SEP), the root mean square error of calibration/prediction (RMSEC/RMSEP) , RPD : the ratio of standard error of prediction (SEP) to standard deviation (SD) and Bias. A high correlation value is an indication that the model may be good; however a high R^2 values does not always result in very good prediction ability. For a good prediction model, it is always desirable to have low prediction error, with fewer latent (optimum) variables to explain the variance while at the same time maintaining a high correlation. The R^2 values for models developed to predict bulk density (kg m^{-3}) and E_d (GPa) of veneer samples using raw spectral data ranged from 0.672-0.761 and 0.561-0.661 respectively for bulk density and stiffness respectively as shown in column 6 of "Tables 1 and 2", and good fit as shown in "Figures 6 and 7".

Table 1: Comparison of PLS models developed for prediction of density (Kg/m^3) of yellow poplar veneer using raw spectra and spectra pre processed with first derivative transformation at different NIR region

	Raw spectra models									First derivative transformed spectra models								
Wavelength (nm)	[1]PC	[2]R^2. Cal.	[3]RMSEC	[4]SEC	[5]R^2 Val	[6]RM SEP	[7]SEP	Bias	*RPD	[1]PC	[2]R2 Cal.	[3]RMSEC	[4]SEC	[5]R^2 Val	[6]RMSEP	[7]SEP	Bias	*RPD
800-2500 (nm)	7	0.758	0.157	0.157	0.761	0.154	0.150	0.036	3.547	5	0.797	0.144	0.144	0.784	0.146	0.146	0.014	3.644
1200-2400 (nm)	6	0.725	0.167	0.167	0.750	0.157	0.154	0.034	3.455	5	0.748	0.159	0.160	0.787	0.145	0.143	0.002	3.720
1800-2400 (nm)	6	0.688	0.181	0.182	0.706	0.171	0.169	0.025	3.148	5	0.716	0.173	0.174	0.742	0.160	0.158	0.029	3.367
1400-2000 (nm)	6	0.645	0.197	0.194	0.672	0.180	0.177	0.037	3.006	3	0.632	0.197	0.198	0.689	0.175	0.173	0.035	3.075

Table 2: Comparison of PLS models developed for prediction of stiffness (GPa) of yellow poplar veneer using raw spectra and spectra pre processed with first derivative transformation at different NIR region

	Raw spectra models									First derivative transformed spectra models								
Wavelength (nm)	[1]PC	[2]R^2 Cal.	[3]RMSEC	[4]SEC	[5]R^2 Val	[6]RMSEP	[7]SEP	Bias	*RPD	[1]PC	[2]R^2 Cal.	[3]RMSEC	[4]SEC	[5]R^2 Val	[6]RMSEP	[7]SEP	Bias	*RPD
800-2500 (nm)	7	0.738	0.040	0.040	0.661	0.046	0.045	0.005	3.222	5	0.760	0.039	0.039	0.720	0.041	0.041	0.003	3.537
1200-2400 (nm)	7	0.703	0.043	0.043	0.662	0.046	0.045	0.006	3.222	3	0.650	0.047	0.047	0.065	0.046	0.046	0.006	3.152
1800-2400 (nm)	6	0.649	0.048	0.048	0.617	0.049	0.048	0.006	3.021	3	0.628	0.049	0.049	0.595	0.050	0.050	0.007	2.900
1400-2000 nm	5	0.587	0.052	0.052	0.561	0.052	0.052	0.007	2.788	3	0.584	0.052	0.052	0.609	0.049	0.049	0.008	2.959

[1]No of principal components,[2] Calibration R^2, [3]Root mean square error of calibration, [4]Standard error of calibration, [5]Validation R^2, [6]Root mean square error of prediction, [7] Standard error of prediction.*Ratio of standard error of prediction to standard deviation (RPD) =SD_y/SEP; where SD_x is the standard deviation of the reference values used in the validation.

RMSEP expressed in the original measurements units provides a measure of the accuracy of prediction model. It expresses the average error expected to be associated with future predictions.

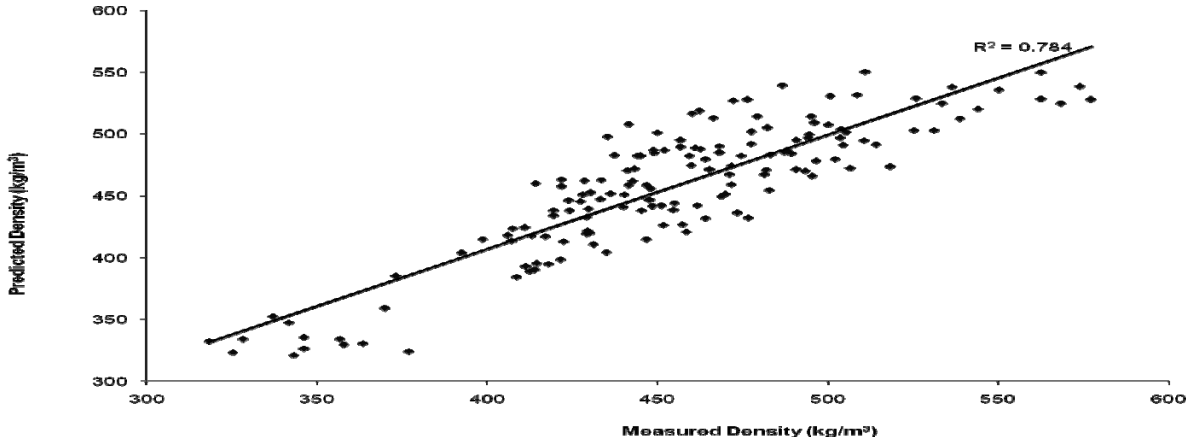

Figure 6: Plot of Measured versus predicted density for model developed with spectra preprocessed with first derivative transformation at wavelength range of 800-2500 nm

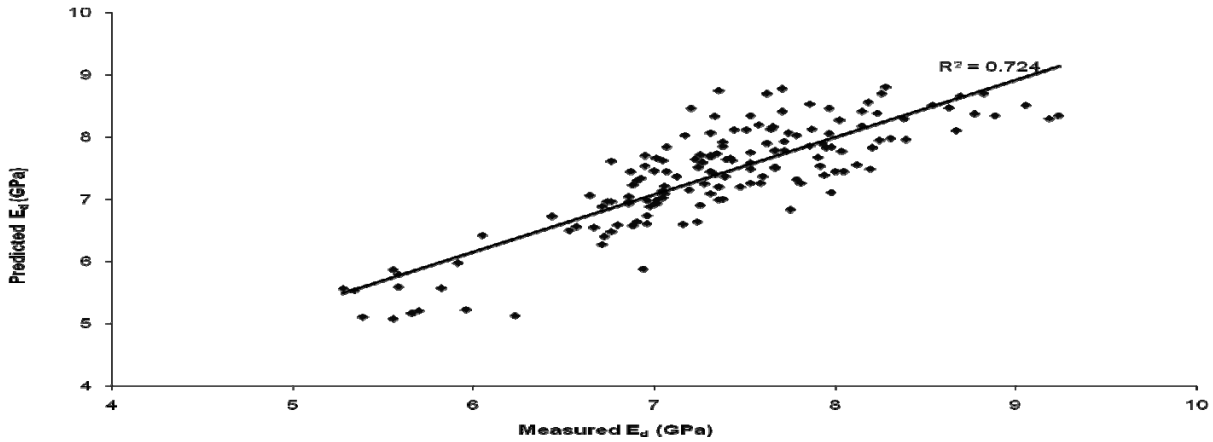

Figure 7: Plot of Measured versus predicted dynamic MOE for model developed with spectra preprocessed with first derivative transformation at wavelength range of 800-2500 nm

Bias represents the average differences between predicted and measured reference values for all samples in the validation set, and it is also used to check if there is a systematic difference between the average values of samples in the calibration and validation set. If there is no such difference, the Bias will be zero (Esbensen 2002). The ratio of SEP to standard deviation (SD), or RPD is a simple statistic that enables the evaluation of SEP in terms of the standard deviation of the reference data. It is calculated by dividing the SD of the reference values in the validation by the SEP (Williams 2004). The SD value of Y1 (bulk density) reference matrix was ±0.53 while the Y2 (E_d) SD value was ±0.145. The RPD values ranged from 3.006-3.547 and 2.788-3.222 for models developed to predict bulk density and E_d (GPa) respectively as shown in column 10 of "Tables 1 and 2". A good model should have SEP value much lower than the SD value and the RPD value higher than 5, however RPD values of 3-4 may be able to verify accurate analysis if the SD is between 0.4-0.5 (Williams 2004). The low SD values of both reference values used in this study is an indication of the low variance in the sample population.

There was significant improvement in the predictive ability of models developed with spectral data pre-treated using the 1st derivative method. The R^2 values for models developed to predict bulk density (kg/m^3) and E_d (GPa) of veneer samples using spectral data pre-treated using 1st derivative method ranged from 0.689-0.784 and 0.609-0.720 respectively for bulk density and stiffness respectively as shown in column 15 of "Tables 1 and 2". The fit is shown in "Figures 6 and 7" for bulk density and stiffness respectively. There were also considerable reductions in the number of latent (optimum) variables needed to attain the minimum residual variance as shown in columns 2 and 11 of "Tables 1 and 2"; and lower RMSEP values as shown in columns 7 and 16. There were also slight increment in the RPD values as shown in columns 10 and 20 of both Table "1 and 2". There was no clear distinction between models developed using the full NIR spectral data and NIR spectral data region of 1200-2400 nm; both NIR data spectral regions had almost the same number of optimum principal component (PC) to give almost the same R^2, SEP and RMSEP values "Tables 1 and 2". The findings of this study showed that the restricted wavelength regions of 1800-2400 and 1400-2000 nm could also be used to developed calibration models, however models developed using the full NIR spectral data

and spectral data region of 1200-2400 nm performed much better than the models developed using the restricted NIR spectra region of 1800-2400 nm and 1400-2000 nm in terms of its repeatability. This may be attributed to the fact that the full NIR spectrum (800-2500 nm) contains features or variables that are subtle and unknown, but are important in predicting both bulk density and stiffness of the veneer samples.
Overall, models developed with the full NIR spectra (800-2500 nm) pre-treated using the 1st derivative method performed best for the prediction of both veneer stiffness and density with low prediction error, with fewer latent (optimum) variables required to explain the variance while maintaining a high correlation value. Since whole spectra were used in the modeling, the multivariate PLS models resulted in better predictive precision of the model when compared to models developed using a restricted spectral region or the traditional univariate calibration (Erikson et al. 1999).
The results obtained in this study are comparable to previous studies (Meder *et al.* 2000) where NIR spectroscopy was used to predict veneer stiffness of sheets of radiata pine (Raw spectral: 35 samples, R^2 =0.59, RMSEP =0.87; 1st derivative spectral: 35 samples. R^2 = 0.72, RMSEP =0.73), though with better model performance. The latter can be ascribed to many factors, which may include the differences in determination of stiffness strength, method of spectra collections, number of samples in calibration sets, differences in validation method, and species of tree used in both studies.

Conclusions

This study demonstrated that NIR spectroscopy coupled with multivariate data analysis can be used to develop predictive models for stiffness and bulk density of plant grade veneer. Models which were developed using the spectral range s 1200 – 2400 nm and 800 – 2400 nm were superior to models limited to the 1800 – 2400 and 1400 – 200 nm regions.

References

1. Meder, R; Thumm, A; and Bier, H. 2002. Veneer stiffness predicted by NIR spectroscopy calibrated using mini-LVL test panels. Holz als Roh- und Werkstoff (60**):** 159-164.
2. Esbensen, K.H.2002. Multivariate data analysis in practice: An introduction to multivariate data analysis and experimental design. CAMO Process AS 5th edition, 598pp
3. Williams, P. 2004. Near-infrared technology- getting the best out of light: A short course in the practical implementation of near-infrared spectroscopy for the user. PDK Grain, Nanaimo, British Columbia, Canada.
4. Eriksson, L; Johansson, E; Kettaneh-Wold, N and Wold, S. 1999. Introduction to multi- and megavariate data analysis using projection methods (PCA & PLS). Umetrics AB, SE90719 Umea, Sweden, 490pp