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RESEARCH ARTICLE

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Prediction of mechanical properties of Chinese fir wood by near infrared spectroscopy

Abstract Mechanical properties and the visible and near infrared (NIR) (350–2500 nm) spectra obtained from longitudinal and transverse face of 155 small clear wood samples of Chinese fir (*Cunninghamia lanceolata*) were measured, and 103 of them were used to establish calibration models. Calibrations were tested on an independent set (52 samples). Differences between calibrations developed by using the longitudinal and transverse face were small. The calibrations developed by using NIR spectra (350–2500 nm) collected from transverse face were slightly inferior to those developed by using NIR spectra collected from longitudinal face. When reducing the spectral range to between 780 and 1050 nm, the calibrations developed by using NIR spectra collected from longitudinal face were slightly inferior to those developed by using NIR spectra collected from transverse face, and reducing the spectral range causes no decrease in the quality of the models developed using NIR spectra collected from transverse face. Partial lease square (PLS) modeling and test showed that calibrations developed using the visible and NIR spectra from transverse and longitudinal faces and calibrations developed by using the reducing spectral range (780– 1050 nm) from the transverse face were moderate, and have a RPD range from 1.51 to 1.90. It is concluded that NIR spectroscopy can be used as an initial screening.

Keywords near infrared (NIR) spectroscopy, Chinese fir, MOE, MOR, partial least-square (PLS)

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1 Introduction

Chinese fir (*Cunninghamia lanceolata*) is a kind of coniferous species distributed in 17 provinces of southern China, with wide distribution and large standing volume. It is known that the physical and mechanical properties of Chinese fir wood vary between standing conditions, and between provenances, families, as well as clones, even vary in different locations in an individual tree (Yu, 2000). With the decrease of wood resources, efficient utilization of wood is becoming a significant approach in relieving wood resources shortage. Assessment of the physical and mechanical properties in existing forests or for tree-breeding purposes requires the measurement of a large number of samples. Therefore, it is of practical significance to find a new, rapid and precise method to measure the mechanical properties of wood.

The NIR spectrum is composed mainly of absorptions based on bonds containing hydrogen atoms (C–H, O–H, N–H) (Lu et al., 2001). Main components of wood are cellulose and lignin, whose molecules have lots of groups containing hydrogen, thus they have abundant absorption in near infrared region. This is the chemical basis of the prediction of wood properties by using NIR spectroscopy. By comparison with conventional methods, NIR spectroscopy is a fast analytical method with lower consumption, which can make an analysis of increment core samples and is helpful to the nondestructive evaluation of the properties of standing trees. In addition, if a proper calibration model is established, prediction of various properties of wood can be made by using NIR spectroscopy. Some researches have been reported successfully to predict the properties of wood rapidly and nondestructively, such as chemical properties (Schimleck et al., 1997), wood density (Thygesen, 1994), elastic modulus of bending (MOE) and bending strength (MOR) (Kelley et al., 2004a, 2004b). In recent years, Chinese Academy of Forestry has begun the research on using NIR spectroscopy technology on wood and achieved preliminary results (Yang et al., 2005; Jiang et al., 2006).

The section used for NIR analysis has effects on the

model results to some extent. In the research of wood density concerning Chinese fir, the effect of calibration models established by the spectra collected from transverse face is better than that of models established by the spectra got from longitudinal face (Jiang et al., 2006). While in the research of wood density concerning loblolly pine, there is little difference between the effect of models established by spectra collected from longitudinal and transverse face (Schimleck et al., 2003). At present, there are no studies in the prediction of mechanical properties of Chinese fir wood with NIR spectroscopy, and also no research concerning the performance differences of calibration models for Chinese fir wood established with spectra collected from longitudinal and transverse face respectively so far.

Price of short wavelength near infrared spectroscopy is much lower than that of the spectroscopy with long wavelength. If accurate prediction of wood properties is done by short wavelength NIR spectra, short-wavelength spectroscopy can be exploited with lower cost in the future. In the research of NIR spectra to predict the mechanical properties of the wood of six coniferous species, Kelly et al. (2004a) has found that these wood properties can be well predicted by short wavelength NIR spectra. However, there is still no report on research of whether or not the mechanical properties of Chinese fir wood can also be better predicted by short wavelength near infrared spectroscopy.

In this study, MOE and MOR of clear specimens of Chinese fir wood were measured and diffuse reflection spectra from each transverse and longitudinal face of wood were acquired by NIR spectroscopy. Then, with the help of chemometrics software, optimal calibration models of MOE and MOR were established by spectra collected from two faces. In addition, influences of section and spectrum range on model performance were analyzed. The purpose of the study is to explore the feasibility of predicting mechanical properties of Chinese fir wood by NIR spectra, especially by the short wavelength spectra collected from transverse and longitudinal face.

2 Materials and methods

2.1 Experiment materials

The 18 Chinese fir (*Cunninghamia lanceolata*) trees were harvested from a 33-year-old stand in the National Forest of Huangshan, Anhui and had an average diameter at breast height of 25 cm and an average height of 17 m.

After air-drying, three or four disks with the length of 0.38 m were cut every 1.6 m from 1.5 m level along every tree. Boards approximately 3 cm wide, and 0.38 m long, were cut from the disk centered on the pith. The boards were then planed to a final thickness of about 2 cm. The final dimensions of the bending samples were 30 cm in the longitudinal direction, 2 cm in the tangential direction, and 2 cm in the radial direction.

All of the samples were conditioned to 12% moisture content prior to testing. After NIR measurement, stiffness, or modulus of elasticity (MOE), and ultimate strength, or modulus of rupture (MOR), of 155 clear wood samples were measured in three-point bending according to Chinese national standards the Method for Determination of the Modulus of Elasticity in Static Bending of Wood (GB 1936.1-1991) and the Method for Determination of the Modulus of Rupture in Static Bending of Wood (GB 1936.2-1991). All of the samples were broken with the load applied against their radial face. All the tests were conducted with a Universal Testing Machine (NMB Co., Japan).

2.2 NIR measurements

The NIR measurements were all made with an Analytical Spectral Devices (ASD) LabSpec® Pro NIR spectrometer at wavelengths between 350–2 500 nm using the default parameters. A bifurcated fiber optic probe oriented at a right angle to the sample surface was used to collect the reflectance spectra. A piece of commercial PTFE (Poly Tetra Fluoro Ethylene) white board was used as the white reference material. For each scanning point, 30 scans were collected and averaged into a single spectrum and 12 spectra were collected for each sample from the radial-longitudinal section, and 4 spectra were collected for each sample from the transverse section. The 12 averaged spectra collected were averaged from the radial-longitudinal section (or 4 averaged spectra as for the transverse section is concerned) to provide a single spectrum that was used to predict the mechanical strength of the individual sample. The NIR spectra of the different species were measured at different time over a one-month period, but all of the samples from one species were measured in one week.

2.3 Mechanical properties determination of wood

Two-third samples (103) were selected as calibration set and 1/3 (52) were selected as prediction set. According to the national standard GB 1927-1943-91, MOE and MOR of calibration set and prediction set were tested. The statistical descriptions of MOE and MOR are shown in Table 1.

2.4 Partial least-squares (PLS) regression

NIR spectra were collected with ASD's Indico data collection and pre-processing software. The spectra were converted to the first-derivative mode to eliminate the influence of instrument background and drifting on signals. Multivariate analysis was performed using Unscrambler version 9.2 software. The models were constructed with the spectral range between 350 and 2500 nm and between 780 and 1050 nm respectively.

Calibrations were developed using PLS-1analysis. The standard error of calibration SEC (determined from the residuals of the final calibration), and the calibration coefficient (R_c) were used to assess calibration performance.

The standard error of prediction (SEP) gave a measure of how well a calibration predicts the properties of unknown samples. Unscrambler software recommended the optimum number of factors to use for calibration, and all of the PLS models were based on 3 to 7 factors.

RPD (ratio of the standard deviation of the reference results to SEP) is a measurement of the predictive ability of an NIR calibration model. Reporting the SEP alone may be misleading unless it is reported by comparison with the standard deviation of the original reference data. If the SEP is close to the SD, then the NIRS calibration is not efficiently predicting the composition or functionality. A RPD of greater than 2.5 is considered satisfactory for screening, although it has been shown that with a RPD of approximately 1.5, NIR spectroscopy can be used as an initial screening tool (Williams and Sobering, 1993; Schimleck et al., 2003; Jones et al., 2005). Determination of the RPD allows comparison of calibrations developed for different wood properties, and the higher the RPD, the more accurate the data fitted by the calibration.

3 Results and discussion

3.1 Variation and pre-processing of NIR spectra

The NIR spectra collected were averaged to give a single spectrum for each specimen. Absorption spectra of longitudinal and transverse face of Chinese fir wood are shown in Fig. 1, while the corresponding first differential diffuse reflection spectra are shown in Fig. 2. As observed from Fig. 1, the average spectra of transverse face have far greater absorbance than that collected from longitudinal face. The reason was that spectra in the transverse face could penetrate into the sample along the tracheids. As a result, reflected energy was relatively low.

Compared between the original spectra (Fig. 1) and the first differential spectra (Fig. 2), it could be found that there was a baseline shift for the original spectra of wood samples, while the processed spectra could eliminate it. In addition, it could also be seen that there was not a significant absorption peak in the original spectra; instead, there were many broad peaks and shoulder peaks in the original spectra. However, the absorption peak of the first differential spectra became steeper and narrow. As a result, the first differential spectra seemed to be easier to analyze.

3.2 NIR Calibrations and predictions

3.2.1 Comparison of calibration using full spectra collected from longitudinal and transverse face

Summary statistics of calibration for MOE and MOR of Chinese fir wood are shown respectively in Tables 2 and 3.

Table 2 shows that the calibration and prediction models of MOE developed using NIR spectra collected from longitudinal face gave slightly improved summary statistics compared with the calibration and prediction models of MOE developed using NIR spectra collected from

Table 1 Statistical description of *C. lanceolata* solid wood MOE (GPa) and MOR (MPa) for the calibration and prediction sets

properties	calibration set				prediction set			
	mean	maximum	minimum	SD	mean	maximum	minimum	SD
MOE	12.39	7.77	17.91	2.14	12.85	9.43	18.49	2.16
MOR	75.24	53.46	104.13	10.39	77.50	52.28	105.31	10.82

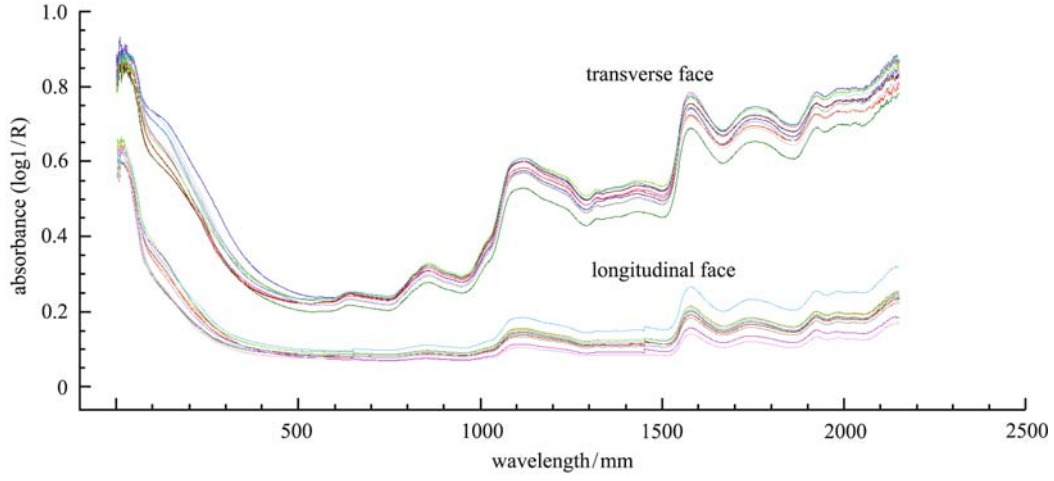

Fig. 1 Variation in NIR absorption spectra collected from longitudinal and transverse face of Chinese fir

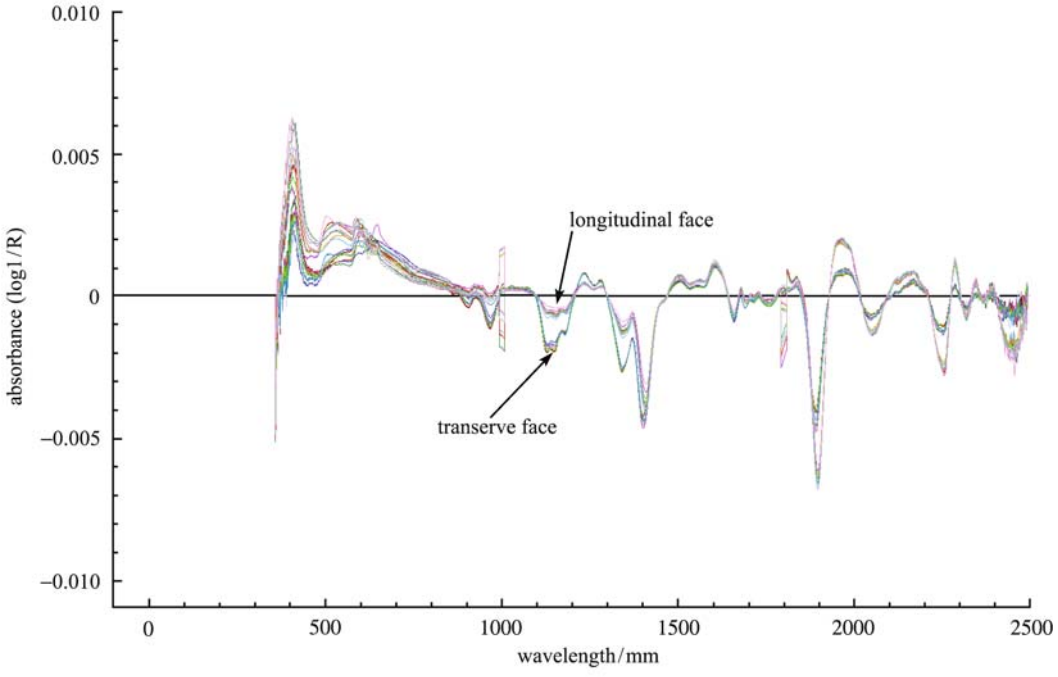

Fig. 2 Variation in first derivatives NIR spectra collected from longitudinal and transverse face of Chinese fir

Table 2 Summary statistics of calibration for *C. lanceolata* solid wood MOE (GPa) (350–2500 nm)

spectrum region	NOPC	calibration set			prediction set	
		R_c	SEC	R_p	SEP	RPD
longitudinal face	7	0.89	0.97	0.79	1.34	1.61
transverse face	5	0.84	1.14	0.75	1.43	1.51

Table 3 Summary statistics of calibration for *C. lanceolata* solid wood MOR (GPa) (350–2500 nm)

spectrum region	NOPC	calibration set			prediction set	
		R_c	SEC	R_p	SEP	RPD
longitudinal face	4	0.91	4.22	0.87	5.70	1.90
transverse face	5	0.92	3.91	0.82	6.47	1.67

transverse face. Their calibration coefficients were 0.89 and 0.84 respectively, and calibration standard errors were 0.97 and 1.14 respectively. While, prediction coefficients were 0.79 and 0.75 respectively, prediction standard errors were 1.34 and 1.43 respectively, as well as RPD of prediction were 1.61 and 1.51 respectively.

Table 3 shows that performance of calibration models of MOR using NIR spectra collected from transverse face was improved than that from longitudinal face. However, performance of prediction models using NIR spectra collected from longitudinal face was slightly improved than that using NIR spectra collected from transverse face. Calibration coefficients of spectra calibration models collected from transverse and longitudinal face were 0.91 and 0.92 respectively, and calibration standard errors were 4.22 and 3.91 respectively. While, prediction coefficients were 0.87 and 0.82 respectively, prediction standard errors were 5.70 and 6.47 respectively, as well as RPD of prediction were 1.90 and 1.67 respectively.

Spectra obtained from transverse face was only from four points, and the scanning position was not on the middle of the specimen where the stress was highest, while spectra obtained from longitudinal face were obtained from 12 points, including the middle point. As a result, in this experiment, spectra obtained from longitudinal face could better reflect the properties variation of specimens, which might be the reason why performance of mechanical properties models established by NIR spectra collected from longitudinal face was better than that from transverse face.

From the above results, it could be seen that there were certain differences between the performance of MOE and MOR models established by spectra data collected from longitudinal face and transverse face. However, RPD was from 1.51 to 1.90, failing to reach 2.50. The ability of predicting MOE and MOR by NIR spectroscopy was not very precise, which could only be used as an initial

screening tool. Testing specimens in this experiment was a little large (2 cm×2 cm×30 cm), considering the variation of wood properties in mind it is true that the collected spectra could not represent the properties of the whole specimen. Thus reducing the size of specimens might further improve the performance of NIR calibration.

3.2.2 Comparison of calibration using short-spectra collected from longitudinal and transverse face

Statistical results of MOE and MOR models established by short-wavelength spectra (780–1050 nm) collected from longitudinal and transverse faces are shown in Tables 4 and 5 respectively. As can be seen in Table 4, Calibration coefficients of MOE models using spectra from transverse and longitudinal face were 0.84 and 0.82 respectively, as well as calibration standard errors were 1.18 and 1.21 respectively. While prediction coefficients were 0.75 and 0.77 respectively, standard errors of prediction were 1.46 and 1.39, RPD were 1.48 and 1.55 respectively. Table 5 shows that Calibration coefficients of MOR models using spectra obtained from transverse and longitudinal face were 0.89 and 0.86 respectively, as well as calibration standard errors were 4.84 and 5.26 respectively. While prediction coefficients were 0.75 and 0.82 respectively, standard errors of prediction were 7.38 and 6.34, RPD were 1.47 and 1.71, respectively.

From the above comparison of Statistical results, it was found that performance of calibration models of MOE and MOR established using spectra collected from longitudinal face was slightly better, while prediction quality of models established using spectra collected from transverse face was slightly better. Repeated training was needed when establishing calibration models and therefore there might have some Over-fitting. However, prediction set was not involved in model calibration, so prediction results might better represent the real prediction ability of the model.

Figure 1 shows that in the spectral range from 780 to 1050 nm, absorption of the spectrum obtained from transverse face was more significant than that from longitudinal face. As can be seen in Fig. 2, the wave trough of the differential spectrum from transverse face was lower and narrower than that from longitudinal face, so the spectrum obtained from transverse face became easier to analyze. This might be the reason that prediction ability of the model established using short wavelength NIR spectra from transverse face was improved.

3.2.3 Effects of reduced spectral range

Summary statistics of MOE models established by spectra of full spectral range and the reduced spectral range obtained from transverse face could be seen in Table 2 and Table 4 respectively. Calibration coefficients were 0.84 and 0.82 respectively, calibration standard errors were 1.14 and 1.21 respectively, prediction coefficients were 0.75 and 0.77 respectively, standard errors of prediction were 1.43 and 1.39 respectively, as well as RPD were 1.51 and 1.55 respectively. As can be seen from Tables 3 and 5, the quality of MOR models using the spectra both with reduced spectral range and full range differ slightly. Calibration coefficients were 0.92 and 0.86 respectively, calibration standard errors were 3.91 and 5.26 respectively, prediction coefficients were both 0.82, standard errors of prediction were 6.47 and 6.34 respectively, as well as RPD were 1.67 and 1.71 respectively.

The above comparison showed that calibration quality of MOE and MOR models established using full spectral range spectra obtained from transverse face was slightly increased than that established using reduced spectral range spectra, while prediction quality of models with reduced spectral range spectra was slightly increased than that established using full spectral range spectra. Both their RPDs were from 1.51 to 1.71, failing to reach to 2.50. As a result, NIR spectroscopy with reduced spectral range obtained from transverse face can be used as an initial screening tool to predict MOE and MOR of Chinese fir wood. As for calibration models established by spectra with reduced spectral range obtained from transverse face, scatter diagrams of NIR-estimated values and measured values of MOE and MOR are shown in Figs. 3 and 4 respectively.

Table 4 Summary statistics of calibration for *C. lanceolata* solid wood MOE (GPa) (780–1050 nm)

spectrum region	calibration set				prediction set	
	number of factors	R_c	SEC	R_p	SEP	RPD
longitudinal face	5	0.84	1.18	0.75	1.46	1.48
transverse face	4	0.82	1.21	0.77	1.39	1.55

Table 5 Summary statistics of calibration for *C. lanceolata* solid wood MOR (GPa) (780–1050 nm)

spectrum region	calibration set				prediction set	
	number of factors	R_c	SEC	R_p	SEP	RPD
longitudinal face	4	0.89	4.84	0.75	7.38	1.47
transverse face	3	0.86	5.26	0.82	6.34	1.71

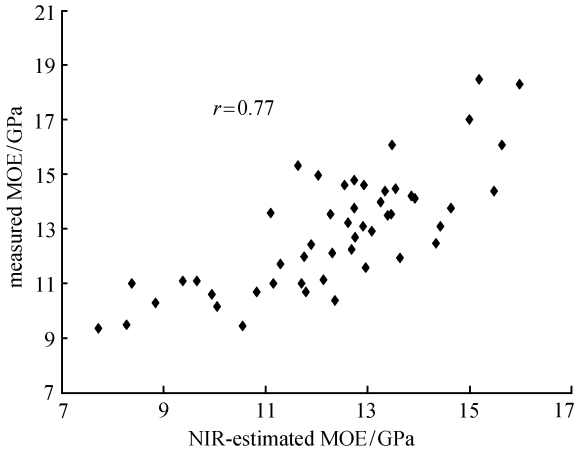

Fig. 3 Correlation between NIR-estimated and measured MOE

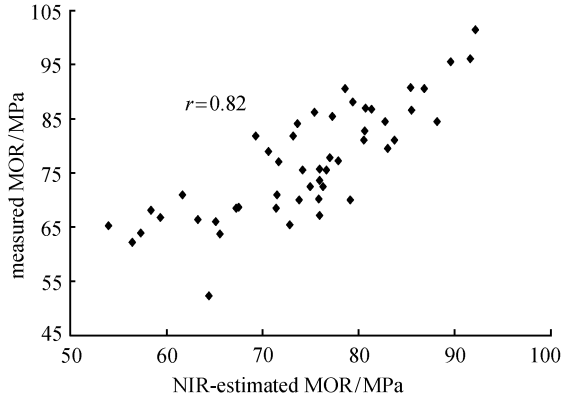

Fig. 4 Correlation between NIR-estimated and measured of MOR

4 Conclusions and discussion

Differences between calibrations developed by using the longitudinal and transverse face were small. The calibrations developed by using NIR spectra (350–2500 nm) collected from transverse face were slightly inferior to those developed by using NIR spectra collected from longitudinal face.

When reducing the spectral range to between 780 and 1050 nm, the calibrations developed by using NIR spectra collected from longitudinal face were slightly inferior to those developed by using NIR spectra collected from transverse face, and reducing the spectral range causes no decrease in the quality of the models developed using NIR spectra collected from transverse face.

Partial lease square (PLS) modeling and test showed that calibrations developed using the visible and NIR spectra from transverse and longitudinal faces and calibrations developed by using the reducing spectral range (780–1050 nm) from the transverse face were moderate, and have a RPD range from 1.51 to 1.90. It is concluded that NIR spectroscopy can be used as an initial screening.

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