

APPLICATION OF NEAR INFRARED SPECTROSCOPY TO A DIVERSE RANGE OF SPECIES DEMONSTRATING WIDE DENSITY AND STIFFNESS VARIATION

by

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SUMMARY

The application of near infrared (NIR) spectroscopy to a large number of mixed species that display extremely wide variations in wood chemistry, anatomy and physical properties, is described. The mixed species samples were characterized in terms of density, longitudinal modulus of elasticity and microfibril angle. NIR spectra were obtained from the radial/longitudinal face of each sample and used to generate calibrations for the measured physical properties. The calibrations developed for density and longitudinal modulus of elasticity had the highest coefficients of determination (R^2) and demonstrated that it is possible to develop general calibrations for these important wood properties across a wide range of species.

The mixed species calibrations were used to estimate wood properties of two species, *Eucalyptus delegatensis* R.T. Baker and *Pinus radiata* D. Don. The results obtained for density and longitudinal modulus of elasticity indicated that mixed species calibrations can be used to rank trees. In practice the extreme variation of samples selected for this study would not be required. It is expected that refinement of calibrations, through sample selection, would provide more accurate prediction of physical properties.

Key words: Near infrared spectroscopy, density, wood stiffness, microfibril angle.

INTRODUCTION

Several studies have demonstrated that near infrared (NIR) spectroscopy can be used to estimate wood properties such as density, wood stiffness (longitudinal modulus of elasticity - E_L) and microfibril angle (MFA). NIR spectroscopy is an analytical technique that has been widely used to rapidly estimate parameters that traditionally have been time consuming and difficult to measure. NIR spectra consist mainly of overtone and combination bands of the fundamental stretching vibrations of O-H, N-H and C-H functional groups and contain chemical and physical information about a sample (Kaye 1954; Shenk et al. 1992). NIR spectroscopic analysis involves measur-

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ing the NIR spectra of a large number of samples, developing a regression calibration that links the spectra to the parameter of interest and then using the calibration and the spectra of a new set of samples to validate the calibration (Martens & Næs 1984; Thomas 1994).

Studies that have used NIR spectroscopy to estimate wood properties have generally been based on solid wood samples of single species such as *Picea abies* (L.) Karsten (Thygesen 1994; Hoffmeyer & Pedersen 1995), *Eucalyptus delegatensis* R.T. Baker (Schimleck et al. 2001a) and *Pinus radiata* D. Don (Schimleck et al. 2001c). Studies have also been based on the milled wood of *Eucalyptus globulus* Labill. subsp. *globulus* (Schimleck et al. 1999; Schimleck & French 2001).

Recently Schimleck et al. (2001b) developed a calibration for wood stiffness which had been estimated using SilviScan-2 data and measured density (Evans & Ilic 2001), using both *E. delegatensis* and *P. radiata* samples (referred to in the remaining text as the *E. delegatensis* + *P. radiata* calibration). The calibration had a strong coefficient of determination (R^2) of 0.88 and fitted the data very well over the range of approximately 5 to 25 GPa. The stiffness of samples greater than 25 GPa was underestimated. Considering that the calibration was developed with species that exhibit large differences in wood chemistry and anatomy (*E. delegatensis* is a hardwood and *P. radiata* is a softwood) the strength of the calibration was surprising. Schimleck et al. (2001b) expressed the opinion that the baseline shift observed between samples of different densities (Schimleck et al. 2001a) was fundamental to the success of the calibration and that the shift was relatively consistent for the two species.

The *E. delegatensis* + *P. radiata* calibration developed by Schimleck et al. (2001b) indicated that it might be possible to produce general NIR calibrations based on samples from a number of different species of a single genus or samples from a number of different genera. The aims of this study were:

- a) to develop calibrations for density, E_L and MFA using NIR spectra obtained from the radial/longitudinal face of samples representing a number of different species, and
- b) to use the density, E_L and MFA calibrations to estimate wood properties of samples from two species, *E. delegatensis* and *P. radiata*.

EXPERIMENTAL

Sample selection

Fifty-nine samples, which had an extremely wide range of wood properties and included many commercially important timber species from around the world, were selected from the CSIRO Forestry and Forest Products H.E. Dadswell wood library. The samples, country of origin and wood properties (density, E_L , MFA and 100/MFA) are given in Table 1.

Fifty *Eucalyptus delegatensis* and forty-nine *Pinus radiata* samples were selected from samples described in Schimleck et al. (2001a, c). The samples were selected to encompass the variation that existed in the *E. delegatensis* and *P. radiata* sets. The wood property data used were the same as that used in Schimleck et al. (2001a, c).

Sample preparation

Dried clear wood samples were equilibrated to approximately 12% moisture content and cut to 20 mm × 20 mm transversely and 300 mm longitudinally. After measurement of E_L , a small strip (2 mm tangentially, 7 mm longitudinally, ~20 mm radially) was cut from one end of each sample for MFA analysis on SilviScan-2 and NIR analysis, as described below.

Wood properties

Dimensions and masses of the dried clearwood test samples (at 12% moisture content) were used to calculate their average air-dry densities (D_{stick}). E_L was determined using the natural frequency of vibration along the fibre direction. A detailed description of this procedure is given in Ilic (2001).

Dimensions and masses of the SilviScan-2 test samples were used to calculate their average air-dry densities (D_{strip}), and MFA was estimated on SilviScan-2 using scanning X-ray diffractometry (Evans 1997, 1999; Evans & Ilic 2001). Schimleck et al. (2001a) found that the relationship between laboratory determined MFA and NIR fitted MFA was not linear for *E. delegatensis*. A simple transformation (100/MFA) was used to give an improved calibration.

Near infrared spectroscopy

NIR diffuse reflectance spectra were obtained from the radial/longitudinal face of each sample using a NIRSystems Inc. Model 5000 scanning spectrophotometer. Samples were held in a custom-made holder (Schimleck et al. 2001a). A 5 mm × 15 mm mask was used to ensure a constant area was tested. The spectra were collected at 2 nm intervals over the wavelength range 1100–2500 nm. The instrument reference was a ceramic standard. Fifty scans were accumulated for each sample and the results averaged. One spectrum was obtained per sample.

The spectra were converted to the second derivative mode (Shenk et al. 1992) for the development of calibrations using the instrument's NSAS[®] software. A segment width of 10 nm and a gap width of 20 nm were used for the conversion.

Calibration

Calibrations were developed for each wood property using Partial Least Squares (PLS) regression. A detailed description of PLS regression is provided by Esbensen et al. (1994). All mixed species samples were used to develop the calibrations. The calibrations were tested on the *E. delegatensis* and *P. radiata* sample sets.

Calibrations were developed using NSAS[®] software (version 3.52). Calibrations were developed with four cross validation segments and a maximum of ten factors. The choice of how many factors to use is very important. NSAS[®] software recommends the optimum number of factors based on the ratio of the mean square error of cross validation (MSECV) for a given factor, to the minimum MSECV obtained for all factors. The software recommends the first factor that gives a ratio of less than 1.25 (Anonymous 1990). In this experiment two factors were recommended for each wood property (apart from MFA where one factor was recommended) but it was observed

Table 1. Species, country of origin and wood properties of the samples used in the study.

Botanical name	Common name	Country of origin	D _{stick} (kg/m ³)	D _{strip} (kg/m ³)	E _L (GPa)	MFA (deg)	100/MFA (deg ⁻¹)
<i>Abies alba</i>	True fir	Europe	416	419.9	10.6	10.7	9.3
<i>Acacia mearnsii</i>	Black wattle	Australia	736	787.4	17.2	12.6	7.9
<i>Agathis robusta</i>	Kauri	Australia	470	484.5	18.3	9.7	10.3
<i>Agathis robusta</i>	Kauri	Australia	493	522.4	12.8	11.9	8.4
<i>Alnus glutinosa</i>	Alder	USA	434	449	10	11.6	8.6
<i>Amora cucullata</i>	Amoora	Papua New Guinea	573	600.6	11.4	13.5	7.4
<i>Atherosperma moschatum</i>	Sassafras	Australia	631	661.8	12.6	14.9	6.7
<i>Athrotaxis selaginoides</i>	King William pine	Australia	387	423	7.1	25.2	4
<i>Beilschmiedia tawa</i>	Tawa	New Zealand	725	733.8	21	10	10
<i>Castanospermum australe</i>	Black bean	Australia	733	722.1	14.8	13.6	7.4
<i>Ceratopetalum apetalum</i>	Coachwood	Australia	677	694.5	22.1	9.4	10.6
<i>Chlorophora excelsa</i>	Iroko	Africa	653	673	15.2	10.9	9.2
<i>Corymbia maculata</i>	Spotted gum	Australia	961	954.7	23.8	9.6	10.4
<i>Dacrydium cupressinum</i>	Rimu	New Zealand	622	627.3	10	19.8	5.1
<i>Daniellia ogea</i>	Ogea	West Africa	727	734.1	18	11.7	8.5
<i>Decussocarpus vitiensis</i>	Salu salu	Fiji	419	411.3	7	22	4.5
<i>Dracontomelum dao</i>	New Guinea walnut	Papua New Guinea	572	577.7	10	12.5	8
<i>Dyera costulata</i>	Jelutong	Malaysia	379	377.5	9.1	11.8	8.5
<i>Dysoxylum muelleri</i>	Queensland rosewood	Australia	753	800	14.3	10.9	9.2
<i>Endiandra palmerstonii</i>	Queensland walnut	Australia	719	740	16	12.6	7.9
<i>Endospermium macrophyllum</i>	Kauvula	Fiji	461	490.9	11.9	12	8.3
<i>Eucalyptus marginata</i>	Jarrah	Australia	949	935	15.9	11.8	8.5
<i>Eucalyptus muellerana</i>	Yellow stringybark	Australia	860	864.5	21.5	9.6	10.4
<i>Eucalyptus obliqua</i>	Messmate	Australia	646	629.4	12.7	15.1	6.6
<i>Eucalyptus ptilularis</i>	Blackbutt	Australia	814	800.5	16.3	10.8	9.3
<i>Eucalyptus sideroxylon</i>	Red ironbark	Australia	1005	1008.2	14.6	12.4	8.1
<i>Fagus sylvatica</i>	European beech	Europe	652	665.7	15.5	12.9	7.8
<i>Flindersia brayleyana</i>	Queensland maple	Australia	582	585.4	13.8	11	9.1
<i>Flindersia schottiana</i>	Silver ash	Australia	694	680.6	20.5	10.6	9.4

(Table 1 continued)

Botanical name	Common name	Country of origin	D _{stick} (kg/m ³)	D _{strip} (kg/m ³)	E _L (GPa)	MFA (deg)	100/MFA (deg ⁻¹)
<i>Gluta reinghas</i>	Malaysian rosewood	Malaysia	624	644.5	18.5	9.1	11
<i>Gonystylus macrophyllus</i>	Ramin	SE Asia	672	691.1	17.1	10.7	9.3
<i>Grevillea robusta</i>	Silky oak	Australia	633	639.2	15.9	10.9	9.2
<i>Intsia bijuga</i>	Merbau	Malaysia	855	885	16.8	14.9	6.7
<i>Juglans nigra</i>	American (black) walnut	USA	562	582.2	10.6	17.7	5.6
<i>Lagarostrobos franklinii</i>	Huon pine	Australia	553	554.5	10.1	20.4	4.9
<i>Lovoa trichilioides</i>	African walnut	West Africa	530	542.7	11.7	12.3	8.1
<i>Myristica chartacea</i>	Fijian cedar	Fiji	609	632.8	16.4	11.2	8.9
<i>Nothofagus fusca</i>	New Zealand beech	New Zealand	640	661.7	17.9	12	8.3
<i>Ochroma lagopus</i>	Balsa	South America	97	108.2	1.7	11.7	8.5
<i>Palaquium amboinense</i>	Pencil cedar	Papua New Guinea	453	465.6	14.7	8.7	11.5
<i>Palaquium spp.</i>	Nyatoh	Malaysia	535	558.9	15.6	11.6	8.6
<i>Paulownia tomentosa</i>	Paulownia	Australia (plantation)	332	354.5	7.2	18.8	5.3
<i>Paulownia tomentosa</i>	Paulownia	Australia (plantation)	303	297.6	6.9	17.6	5.7
<i>Phyllocladus asplenifolius</i>	Celery top pine	Australia	494	492	11.3	17.6	5.7
<i>Phyllocladus asplenifolius</i>	Celery top pine	Australia	627	658.4	15.6	13.4	7.5
<i>Picea sitchensis</i>	Sitka spruce	Canada	398	419.7	13.2	12.7	7.9
<i>Pinus lambertiana</i>	Sugar pine	USA	445	525.5	11	10.7	9.3
<i>Pinus sylvestris</i>	Baltic pine	Europe	553	564.8	18.2	10.1	9.9
<i>Pinus sylvestris</i>	Baltic pine	Europe	605	616.2	17.4	12.1	8.3
<i>Pterocarpus indicus</i>	New Guinea rosewood	Papua New Guinea	514	537.4	11.2	12.4	8.1
<i>Quercus alba</i>	American oak	USA	706	691.1	13.9	13.7	7.3
<i>Sindora sumatrana</i>	Sepiter	Malaysia	674	679	17.3	9.6	10.4
<i>Swietenia macrophylla</i>	Brazilian mahogany	Central/S. America	600	598.6	13.2	13.1	7.6
<i>Syncarpia glomulifera</i>	Turpentine	Australia	912	918.1	15.6	10.8	9.3
<i>Tectona grandis</i>	Teak	Myanmar	675	689.3	15.1	11	9.1
<i>Thuja plicata</i>	Western red cedar	Canada/USA	371	395.4	6.2	11.7	8.5
<i>Thuja plicata</i>	Western red cedar	Canada/USA	349	348.3	6.3	17.9	5.6
<i>Toona sureni</i>	Philred cedar	Philippines	410	436.3	10.3	10.4	9.6
<i>Ulmus japonica</i>	Japanese elm	Japan	614	603.3	12	20.4	4.9

that the ratio of MSECV to minimum MSECV was less than 1.25 for several additional factors. For D_{stick} and D_{strip} the ratio was less than 1.25 from factors two to six, for MOE factors two to seven, for MFA factors one to ten and for 100/MFA factors two to ten. Results are reported for all calibrations that had ratios of less than 1.25 apart from MFA and 100/MFA where the results are only reported up to the sixth factor, as additional factors did not improve predictions made by the calibrations.

Calibration statistics

The measure of how well a calibration fits the data is the Standard Error of Calibration (SEC). The measure of how well the calibration predicts the constituent of interest for a set of unknown samples that are different from the calibration test set is given by the Standard Error of Prediction (SEP). Formulas used to estimate the SEC and SEP are given in Schimleck et al. (2001a).

Table 2. Summary statistics of the mixed species stick density (D_{stick}) calibrations and of predictions made by these calibrations on the *E. delegatensis* and *P. radiata* sample sets. MSECV is the mean square error of cross validation, SEC is the standard error of calibration and SEP is the standard error of prediction.

# of factors	Mixed species calibration			<i>E. delegatensis</i>		<i>P. radiata</i>	
	MSECV / MSECV (min)	R ²	SEC	R ²	SEP	R ²	SEP
2	1.00	0.76	87.2	0.41	109.0	0.57	90.8
3	1.04	0.81	79.4	0.59	75.5	0.64	44.5
4	1.10	0.82	76.2	0.72	65.8	0.67	39.4
5	1.12	0.85	72.0	0.69	71.9	0.62	45.1
6	1.19	0.86	69.1	0.67	84.0	0.62	53.8

Table 3. Summary statistics of the mixed species strip density (D_{strip}) calibrations and of predictions made by these calibrations on the *E. delegatensis* and *P. radiata* sample sets. MSECV is the mean square error of cross validation, SEC is the standard error of calibration and SEP is the standard error of prediction.

# of factors	Mixed species calibration			<i>E. delegatensis</i>		<i>P. radiata</i>	
	MSECV / MSECV (min)	R ²	SEC	R ²	SEP	R ²	SEP
2	1.00	0.76	86.0	0.43	112.0	0.68	97.5
3	1.04	0.81	77.2	0.65	72.8	0.77	49.4
4	1.16	0.83	74.0	0.75	65.4	0.79	40.0
5	1.16	0.85	70.0	0.72	70.4	0.75	34.7
6	1.22	0.87	66.9	0.70	82.0	0.75	40.3

RESULTS

D_{stick} and D_{strip} calibrations

The calibrations developed for D_{stick} and D_{strip} and the results obtained when these calibrations were used to predict the stick and strip density of the *Eucalyptus delegatensis* and *Pinus radiata* sample sets are given in Tables 2 and 3.

Calibrations developed for D_{stick} and D_{strip} had similar coefficients of determination (R^2) and SECs. The two sets of calibrations were very similar because the strips that were used to obtain the spectra represented very well the sticks from which they were cut (R^2 for the linear relationship between D_{stick} and $D_{strip} = 0.99$). The statistics of the D_{strip} calibrations were slightly better than for the D_{stick} calibrations (i.e., lower SEC and SEPs) because the NIR spectra used to develop both stick and strip calibrations were obtained from the surface of the strips and therefore the spectra related directly to the measured strip density.

The mixed species D_{stick} and D_{strip} calibrations had R^2 values that were comparable to those reported for *E. delegatensis* and *P. radiata* (Schimleck et al. 2001a, c), while the SECs were considerably higher. When comparing these statistics it is important to consider the range of the calibration. Compared to the mixed species sample set, the range of densities for *E. delegatensis* and *P. radiata* was narrow (Evans & Ilic 2001; Schimleck et al. 2001c) and hence a lower SEC can be expected for these sets. A plot of laboratory determined D_{stick} versus NIR fitted D_{stick} for the four factor calibration, which gave the best results when used on the *E. delegatensis* and *P. radiata* sample sets, is given in Figure 1. Note that the regression line has been plotted for all figures.

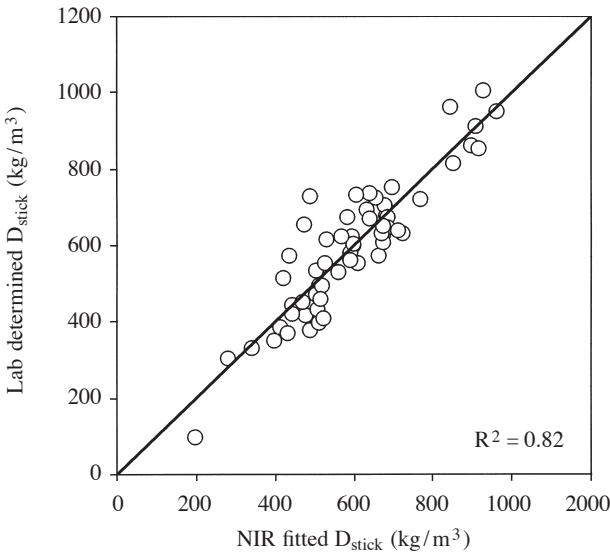


Fig. 1. Relationship between laboratory determined stick density (D_{stick}) and NIR fitted D_{stick} for the four factor mixed species calibration.

Examination of Figure 1 shows that relationship between laboratory determined D_{stick} and NIR fitted D_{stick} was good ($R^2 = 0.82$) considering the extremely wide range of wood chemistries and anatomies represented. There are some samples that are a considerable distance from the regression line, these samples contributed to the high SEC. Eight samples were found to have residuals greater than 100 kg/m^3 and two of

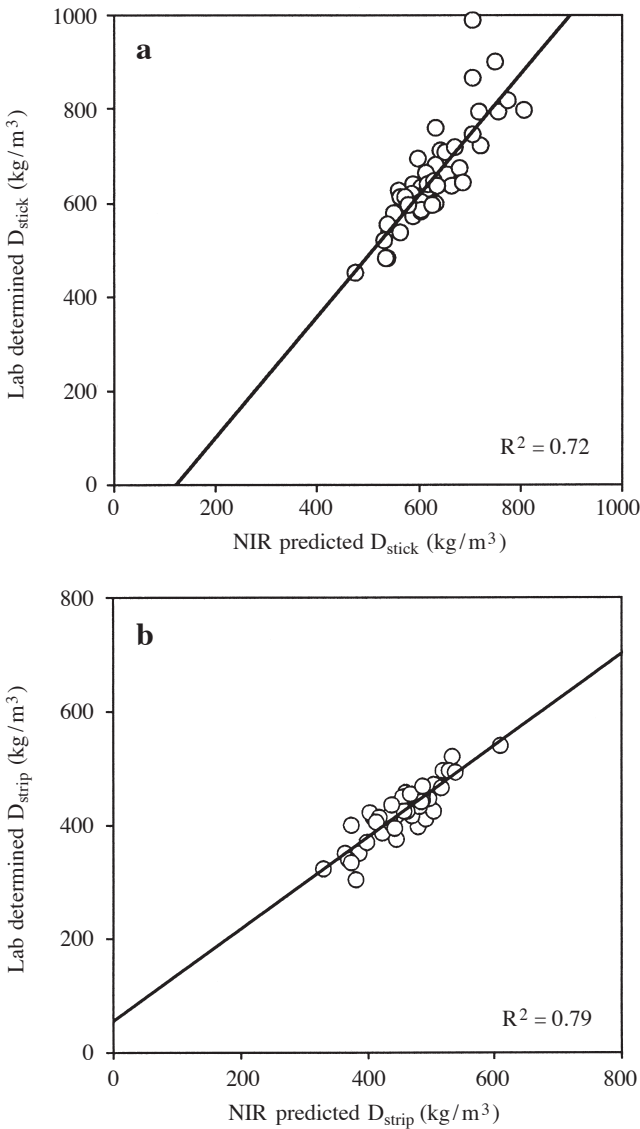


Fig. 2. Relationships between laboratory determined density and NIR predicted density for the *E. delegatensis* samples (D_{stick}) (a) and the *P. radiata* samples (strip density (D_{strip})) (b). Predictions were made using the four factor mixed species D_{stick} and D_{strip} calibrations.

these had residuals greater than 150 kg/m^3 (the residual = NIR fitted value - laboratory determined value). The two samples were *Chlorophora excelsa* (Welw.) Benth. et Hook. f. (-173.6 kg/m^3) and *Daniellia ogea* Rolfe ex Holl. (-226.7 kg/m^3). When the NIR spectra of *C. excelsa* and *D. ogea* were compared with samples of similar density it was found that both species had spectra of lower absorbance than the spectra of the other samples. *Chlorophora excelsa* and *Daniellia ogea* contain high levels of extractives, which may have an influence on their NIR spectra. Calibrations developed using extractives free wood may provide improved results for these species and will be investigated.

When the D_{stick} calibrations were used on the *E. delegatensis* and *P. radiata* sample sets the four factor calibration gave the best results for both species. In comparison, the two factor calibrations recommended by the software gave poor estimates of both the stick and strip densities. Generally the density of the *E. delegatensis* samples were well predicted by the four factor calibration but estimates were poor for samples with high density (Fig. 2a). The highest density *E. delegatensis* sample (990 kg/m^3) had a very large residual (-283.4 kg/m^3). If this sample was removed from the *E. delegatensis* sample set, the R^2 improved to 0.77 while the SEP dropped to 52.4 kg/m^3 . Generally the density of the *P. radiata* samples was overestimated by the mixed species calibration. Despite most samples having their densities overestimated one sample was observed to have a large negative residual (-79.4 kg/m^3). Previously Schimleck et al. (2001c) had reported that three *P. radiata* samples had strip and stick densities that were quite different. The sample identified in this study as having a large negative residual was one of those three samples and if removed from the *P. radiata* set the R^2 improved to 0.76 and the SEP dropped to 38.1 kg/m^3 .

When the D_{strip} calibrations were used on the *E. delegatensis* sample set, the results were similar to those obtained using the D_{stick} calibrations, four factors again gave the best predictions. The highest density sample was again observed to have a large residual (-232.2 kg/m^3), if this sample was removed the R^2 improved to 0.77, while the SEP dropped to 52.4 kg/m^3 . Predictions of *P. radiata* strip density gave similar SEPs but the R^2 were much higher regardless of the number of factors used. Four factors gave the highest R^2 (0.79) but five factors gave the lowest SEP (34.7 kg/m^3). A plot of laboratory determined D_{stick} versus NIR fitted D_{stick} for the four factor calibration is shown in Figure 2b. Differences between predictions of *P. radiata* stick and strip densities were due to the strips not representing the sticks as well as they did for the *E. delegatensis* samples (R^2 for the linear relationship between *P. radiata* D_{stick} and $D_{\text{strip}} = 0.80$, *E. delegatensis* $R^2 = 0.98$).

E_L calibrations

E_L mixed species calibrations and results obtained when these calibrations were used to predict the E_L of the *E. delegatensis* and *P. radiata* samples are given in Table 4. The E_L calibrations had lower R^2 than the density calibrations for a given number of factors. The SEC ranged from 2.81 (two factors) to 2.14 GPa (seven factors) and was higher than the E_L obtained for single species calibrations developed using *E. delegatensis* (four factors recommended, SEC = 1.51GPa) (Schimleck et

Table 4. Summary statistics of the mixed species longitudinal modulus of elasticity (E_L) calibrations and of predictions made by these calibrations on the *E. delegatensis* and *P. radiata* sample sets. MSECV is the mean square error of cross validation, SEC is the standard error of calibration and SEP is the standard error of prediction.

# of factors	Mixed species calibration			<i>E. delegatensis</i>		<i>P. radiata</i>	
	MSECV / MSECV (min)	R ²	SEC	R ²	SEP	R ²	SEP
2	1.07	0.61	2.81	0.68	5.25	0.62	3.10
3	1.00	0.66	2.63	0.66	4.20	0.67	2.52
4	1.07	0.69	2.53	0.67	4.14	0.66	1.82
5	1.08	0.74	2.34	0.71	3.47	0.71	1.26
6	1.19	0.77	2.22	0.70	3.63	0.72	1.26
7	1.20	0.79	2.14	0.76	3.00	0.75	1.18

2001a) and *P. radiata* (two factors recommended, SEC = 1.01 GPa) (Schimleck et al. 2001c). As for density, the wide E_L range of the mixed species contributed to the higher SEC. The *E. delegatensis* + *P. radiata* calibration developed for SilviScan estimated stiffness had a similar range. A three factor calibration was reported that had an SEC of 1.96 GPa (Schimleck et al. 2001b).

When the E_L calibrations were applied to the individual sample sets, the seven factor calibration (Fig. 3) gave the best results for both species. Three samples had large residuals for this calibration, i.e., *Daniellia ogea* (-4.3 GPa), *Atherosperma moschatum* Labill. (4.2 GPa) and *Sindora sumatrana* Miq. (-4.1 GPa).

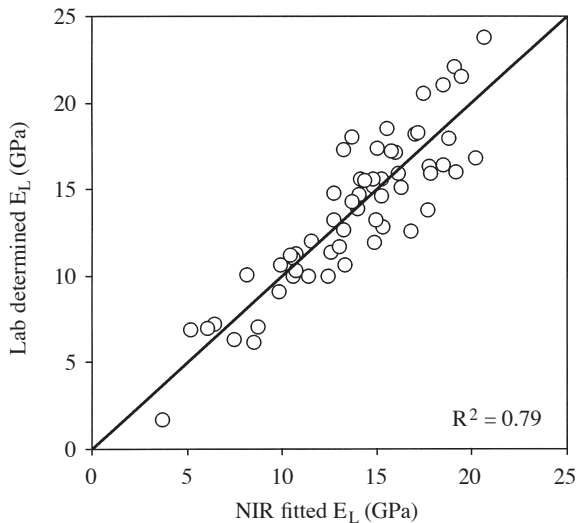


Fig. 3. Relationship between laboratory determined longitudinal modulus of elasticity (E_L) and NIR fitted E_L for the seven factor mixed species calibration.

Large improvements in the SEP were obtained as additional factors were used, particularly for the *E. delegatensis* set. For example, the SEP dropped from 5.25 GPa using two factors to 3.0 GPa using seven factors. Plots of laboratory determined E_L versus NIR predicted E_L for the *E. delegatensis* and *P. radiata* samples are shown in Figure 4.

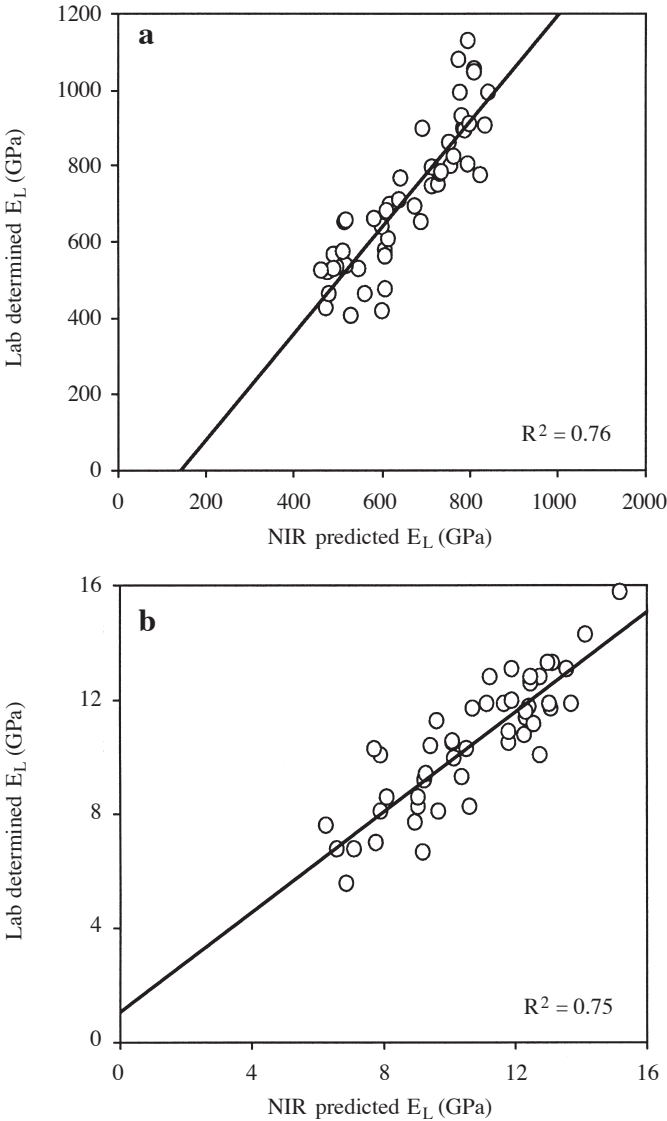


Fig. 4. Relationships between laboratory determined E_L and NIR predicted E_L for the *E. delegatensis* samples (a) and the *P. radiata* samples (b). Predictions were made using the seven factor mixed species E_L calibration.

Generally the mixed species calibration predicted E_L quite well for the *E. delegatensis* set, but it tended to underestimate E_L when greater than 20 GPa and the residuals became greater as E_L increased. The range of E_L in the mixed species calibration was 1.7 to 23.8 GPa and six *E. delegatensis* samples had E_L values beyond the range of the calibration, explaining the poor predictions. If these samples were removed the R^2 dropped to 0.75 but the SEP fell to 2.14 GPa. Predictions of E_L for the *P. radiata* samples were in close agreement with the reference data.

MFA and 100/MFA calibrations

The mixed species MFA and 100/MFA calibrations and the results obtained when these calibrations were used on the *E. delegatensis* and *P. radiata* sample sets are given in Tables 5 and 6.

Table 5. Summary statistics of the mixed species microfibril angle (MFA) calibrations and of predictions made by these calibrations on the *E. delegatensis* and *P. radiata* sample sets. MSECV is the mean square error of cross validation, SEC is the standard error of calibration and SEP is the standard error of prediction.

# of factors	Mixed species calibration			<i>E. delegatensis</i>		<i>P. radiata</i>	
	MSECV / MSECV (min)	R ²	SEC	R ²	SEP	R ²	SEP
2	1.06	0.36	2.86	0.58	2.03	0.58	4.62
3	1.00	0.41	2.75	0.61	1.91	0.55	3.98
4	1.06	0.50	2.58	0.54	2.30	0.60	3.22
5	1.07	0.52	2.53	0.54	2.19	0.63	3.10
6	1.06	0.59	2.35	0.49	2.36	0.63	3.05
7	1.08	0.70	2.05	0.45	2.56	0.59	3.35

Table 6. Summary statistics of the mixed species 100 divided by microfibril angle (100/MFA) calibrations and of predictions made by these calibrations on the *E. delegatensis* and *P. radiata* sample sets. MSECV is the mean square error of cross validation, SEC is the standard error of calibration and SEP is the standard error of prediction.

# of factors	Mixed species calibration			<i>E. delegatensis</i>		<i>P. radiata</i>	
	MSECV / MSECV (min)	R ²	SEC	R ²	SEP	R ²	SEP
2	1.12	0.39	1.38	0.66	1.40	0.55	1.96
3	1.07	0.45	1.32	0.65	1.34	0.48	1.44
4	1.07	0.51	1.25	0.63	1.27	0.53	1.04
5	1.05	0.53	1.23	0.66	1.18	0.56	0.99
6	1.07	0.62	1.13	0.63	1.21	0.61	0.92
7	1.05	0.67	1.05	0.58	1.29	0.55	0.99

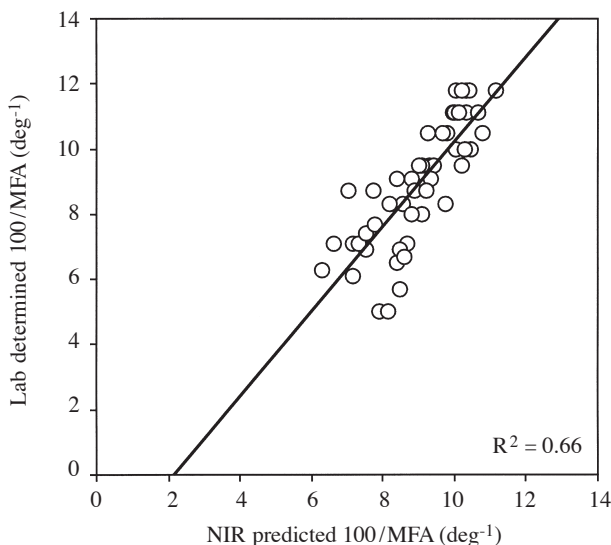


Fig. 5. Relationship between laboratory determined 100 divided by microfibril angle (100/MFA) and NIR predicted 100/MFA for the *E. delegatensis* samples. Predictions were made using the five factor mixed species 100/MFA calibration.

The MFA and 100/MFA calibrations were similar but had poorer calibration statistics than the calibrations developed for density and E_L . Compared to the MFA and 100/MFA individual species calibrations developed for *E. delegatensis* and *P. radiata* (Schimleck et al. 2001a, c) the statistics were inferior for an equivalent number of factors.

When the two sets of calibrations were applied to the *E. delegatensis* set the best predictions for MFA and 100/MFA were obtained using three and five factors respectively. A plot of laboratory determined 100/MFA versus NIR predicted 100/MFA for the five factor calibration is shown in Figure 5. Three samples that had relatively low 100/MFAs (high MFAs) were observed to have large residuals. If these samples were removed the R^2 improved to 0.71 and the SEP dropped to 0.96. For the *P. radiata* set the best results for MFA were obtained using five factors and for 100/MFA six factors gave the best predictions.

DISCUSSION

The results presented in this study demonstrate that it is possible to develop general calibrations for important wood properties using a wide range of species that display extreme variation in wood chemistry, anatomy and physical properties. In addition, the calibrations can be used on separate test sets, in this study comprising single species, to rank trees. The results obtained for D_{stick} , D_{strip} and E_L were particularly promising. The ability to rank these trees demonstrates that differences in NIR spectra due to changes in sample density are relatively consistent for spectra obtained

from the radial/longitudinal face of solid wood samples. Some species, such as *Chlorophora excelsa* and *Daniellia ogea*, did not fit the calibration as well as the other species and this may be due to the high extractives contents of these samples. It is expected that calibrations based solely on these species would be as successful as other individual species calibrations.

The samples selected for this study represent an extreme range and it is improbable that such wide variation would be required in practice. For most applications, samples from a small number of species would probably suffice, for example calibrations based solely on *Eucalyptus nitens* and *Eucalyptus globulus* subsp. *globulus* would satisfy the requirements of nearly all eucalypt plantations in South Eastern Australia. Alternatively, calibrations could be developed for hardwoods, softwoods or trees from a given area. It is expected that refinement of calibrations through appropriate sample selection would provide improved calibration statistics, owing to less variation in the calibration set, and more accurate predictions of the physical properties of test samples.

An additional finding of this study was that the number of factors used for a calibration, as recommended by the software, does not necessarily provide the best predictions. An excellent example was provided by the calibrations developed for density. The two factor D_{strip} calibration (recommended by the software) gave an R^2 of 0.43 and an SEP of 112 kg/m³ when used on the *Eucalyptus delegatensis* set. When the five factor calibration was used the R^2 improved to 0.75 and the SEP fell to 65.4 kg/m³. If only the two factor calibration had been used it would have appeared that the mixed species calibration could not rank trees based on density. If the mixed species D_{strip} calibration was applied to a new sample set comprised of a different species it is impossible to know how many factors would be appropriate. Based on the results obtained for *E. delegatensis* and *Pinus radiata* the four factor calibration would probably be the best, but this may not be the case for a different species. The only way to be sure is to test a selection of samples from the test set and investigate which calibration gives the best predictions. As more sets were tested the calibration that gave the best predictions on average could be selected and used with confidence, negating the need to test subsets of samples.

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