Comparison of wood property calibrations developed using whole-tree and increment core NIR spectra

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Introduction

Aracruz Celulose SA is the largest producer of bleached eucalypt market pulp in the world. The pulp is used to manufacture tissue products and printing and writing papers. The pulp is mainly produced from *Eucalyptus grandis* x *E. urophylla* hybrids that have been selected for their growth and pulp properties. Selection of the most suitable hybrids for propagation is important and many wood quality traits related to pulp production must be considered. For these characteristics to be effectively considered in the selection process, operational techniques that permit rapid, inexpensive and preferably non-destructive evaluation of a large number of individuals in the field is important.

Several studies have demonstrated that near infrared (NIR) spectroscopy can be used to determine wood quality traits related to pulp production.[1–4] These studies have examined the relationships between whole-tree data and NIR spectra obtained from milled chip samples that represent the whole-tree. While the calibrations are strong they can only be applied, with confidence, to other whole-tree composite samples requiring further destructive sampling. An option is to develop calibrations using whole-tree data from destructively sampled trees and NIR spectra collected from increment cores. While calibration development requires destructive sampling to obtain whole-tree data, once developed the calibration can be applied with confidence to increment cores, allowing non-destructive sampling. The approach described has not been investigated and the aim of this study was to examine the relationships between a range of traits and NIR spectra obtained from whole-tree composite chip samples and between NIR spectra obtained from 5 mm increment cores removed from two heights (0.65 and 1.30 m).

Materials and methods

Sample origin

One hundred selected trees that demonstrated wide genetic variation were destructively sampled and chipped to give whole-tree composites. Increment cores (5 mm in diameter) were also removed from these trees at sampling heights of 0.65 and 1.30 m.

Sample preparation

All samples were air-dried. A sub-sample of each whole-tree composite and the increment cores from 0.65 and 1.30 m were milled in a Wiley mill and then in an Udy mill. The samples were milled in the Udy mill to maximise sample recovery from the 5 mm cores.

Determination of wood quality traits

Several wood quality traits were determined on the whole-tree chip samples using published standard methods were possible. Traits included basic density (Tappi T258 om-94), screened pulp yield, soda (NaOH) charge, specific consumption, total lignin (Tappi T222 om-98) and pentosans (Tappi T223 cm-84).

Near infrared spectroscopy

The wood meal was placed in a NIRSystems large sample cup (NR-7070). The NIR spectra were measured in diffuse reflectance mode from samples held in a spinning sample holder in a NIRSystems Inc. Model 5000 scanning spectrophotometer. 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. After the spectrum had been obtained, the sample cup was emptied, repacked and a duplicate spectrum obtained.

The duplicate spectra were averaged and converted to the second derivative using the instrument's Vision software (version 2.31). A segment width of 10 nm and a gap width of 20 nm were used for the conversion.

Calibration development

Calibrations were developed for the whole-tree composites and core samples using partial least squares (PLS) regression. A detailed description of PLS regression is provided elsewhere.[5] The calibrations were developed using Vision software, with four cross validation segments and a maximum of ten factors. The Vision software recommended the final number of factors to use.

Calibration statistics

The measure of how well a calibration fits the data is the standard error of calibration (*SEC*).[6] The co-efficient of determination (R^2) was also used to assess calibration performance.

Results and discussion

Whole-tree composite sample calibrations

Calibrations were developed for each trait using the whole-tree data and NIR spectra obtained from whole-tree composite samples. Calibrations developed for basic density, NaOH charge, pentosans, pulp yield, specific consumption and lignin are reported in Table 1.

Table 1. Summary of calibrations developed for selected wood quality traits using whole-tree data and whole-tree composite samples. *Note 5 factors could be used for the pulp yield calibration, giving a R^2 = 0.51 and an *SEC* = 1.09.

Trait	# of factors	R^2	*SEC*	Deleted samples
Basic density	2	0.72	31.5	3
NaOH charge	2	0.62	0.42	2
Pentosans	3	0.73	0.84	1
Pulp yield*	3	0.37	1.23	4
Specific consumption	2	0.70	0.27	5
Total lignin	3	0.79	0.80	4

Calibrations developed for all traits (apart from pulp yield) using the whole-tree chip samples gave good calibration statistics. Plots showing calibrations developed for pentosans and total lignin are given in Figures 1a and 1b. Both figures show that the pentosans and total lignin calibration data was well fitted by the calibrations.

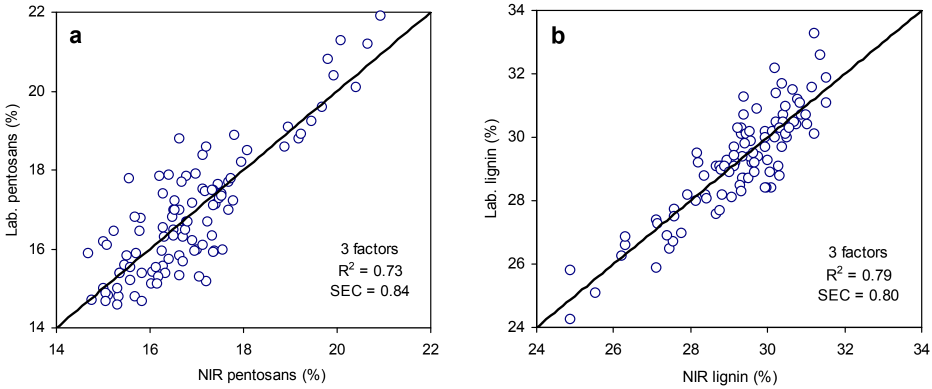

Figure 1. Calibrations developed using NIR spectra collected from whole-tree composite samples and whole-tree data for (a) pentosans and (b) total lignin.

The calibration developed for basic density had a lower R^2 compared to most basic density calibrations published in the literature, but generally strong calibrations have been obtained using solid wood.[7–9] Studies based on milled wood have provided both weaker[10] and stronger[11] relationships. Calibrations developed for pentosans and total lignin compare well with those reported in other studies.[2,12–15] The R^2 reported for NaOH charge and pulp yield calibrations were lower than reported by other authors.[1–3,13,15,16] As far as the authors are aware there are no examples of specific consumption calibrations reported in the literature but calibrations have been published for pulpwood productivity (where pulpwood productivity is equal to pulp yield multiplied by basic density), a comparable trait, and higher R^2 were obtained.[11]

0.65 m core calibrations

Calibrations developed for basic density, NaOH charge, pentosans, pulp yield, specific consumption and lignin using NIR spectra obtained from the 0.65 m cores are reported in Table 2.

Table 2. Summary of calibrations developed for selected wood quality traits using 5 mm cores obtained from a sampling height of 0.65 m.

Trait	# of factors	R^2	*SEC*	Deleted samples
Basic density	4	0.76	29.4	1
NaOH charge	2	0.34	0.55	-
Pentosans	3	0.78	0.76	1
Pulp yield	3	0.57	0.98	2
Specific consumption	2	0.65	0.30	4
Total lignin	3	0.74	0.86	4

Calibrations developed for basic density, pentosans, specific consumption and total lignin all provided good calibration statistics. For basic density and pentosans the calibration statistics were actually improved when the 0.65 m core samples were used but it is important to note that an additional two factors were used for the basic density calibration. The pulp yield calibration provided stronger statistics (Figure 2) but unfortunately the R^2 (0.57) was still low. These calibrations could potentially be used for ranking purposes. The calibration developed for NaOH charge was poor and could not be used to rank trees.

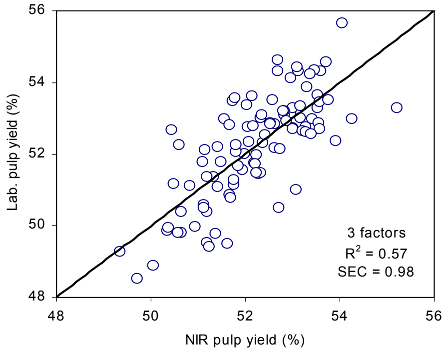

Figure 2. Calibration developed using NIR spectra collected from 0.65 m increment cores and whole-tree data for pulp yield.

1.30 m core calibrations

Calibrations developed for basic density, NaOH charge, pentosans, pulp yield, specific consumption and lignin using NIR spectra obtained from the 1.30 m cores are reported in Table 3.

Table 3. Summary of calibrations developed for selected wood quality traits using 5 mm cores obtained from a sampling height of 1.30 m.

Trait	# of factors	R^2	*SEC*	Deleted samples
Basic density	6	0.78	28.9	25
NaOH charge	1	0.18	0.61	
Pentosans	3	0.75	0.81	94
Pulp yield	3	0.50	1.05	8, 96
Specific consumption	2	0.61	0.31	25, 71, 80, 96
Total lignin	2	0.74	0.87	5, 78

Generally the calibrations developed using the 1.30 m cores were very similar to those developed using the 0.65 m cores and potentially all calibrations, apart from the calibration developed for NaOH charge, could be used for ranking purposes.

Validation of calibrations

The work reported here is ongoing and it is planned to validate all calibrations by testing them on a separate test set.

Identification of a suitable sampling height

For the nondestructive sampling of standing trees it is important that a suitable sampling height be identified. In this study two sampling heights were examined (0.65 and 1.30 m) and the selection of the most appropriate sampling height was based on three criteria:

- The success of calibrations developed for selected traits using core samples from 0.65 and 1.30 m.
- Mahalanobis distance measurements made on NIR spectra of the 0.65 and 1.30 m core samples using a whole-tree chip sample PCA model.
- Practical implications of core sampling at 0.65 and 1.30 m.

Generally the calibrations developed using core samples from 0.65 m gave slightly better calibration statistics than those developed using cores from 1.3 m but the differences were small hence both heights could be used. Of the two heights 1.3 m is by far the most practical and Mahalanobis distances for this height were also more similar to the whole-tree chips. Consequently 1.30 m was identified as the most suitable sampling height.

Conclusions

Calibrations were developed for a range of wood quality traits using NIR spectra obtained from whole-tree composite chip samples. Calibrations developed for basic density, NaOH charge, pentosans, specific consumption and total lignin were good while the calibration developed for pulp yield was poor.

Calibrations were developed for all traits using NIR spectra obtained from the 0.65 and 1.30 m cores and whole-tree data. The calibrations developed for basic density, pentosans, specific consumption and total lignin were very similar to those developed using the whole-tree composite chips. The calibrations developed for pulp yield had superior statistics to those reported for the whole-tree chips. The calibrations for these traits could potentially be used for ranking purposes. The calibrations developed for NaOH charge were poor and could not be used for ranking trees.

1.30 m was identified as the most suitable sampling height. The decision was based on the NIR calibrations developed using the 0.65 and 1.30 m increment cores, Mahalanobis distance measurements and the practicalities of core sampling at the two heights.

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