An efficient method to reduce grain angle influence on NIR spectra for predicting extractives content from heartwood stem cores of *Toona. sinensis*

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Research

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Abstract

Background A fast and reliable non-destructive method for qualifying the content of extracts content (EC) in heartwood of *T. sinensis* cores is needed in the breeding program for studying the genetically infect on EC. However, the affecting of grain angle on near infrared (NIR) spectra prediction model for EC is unclear. In this study, NIR spectra were collected both from cross section and radial section of wood core samples in order to predict the EC in heartwood.

Results The effect of grain angle on calibration EC model was studied. Several different spectra pre-processing methods were tested for calibration. It was found that standard normal variation (SNV) followed by 1 st derivative yield the best calibration for EC. Grain angle has a significant influence on the predict model for EC when use the whole NIR spectra. However, after using the significant multivariate correlation (sMC) selection of the prior of wavenumbers for EC, the influence of grain angle have been significantly reduced.

Conclusions It was suggested that NIR spectroscopy could be a promising methods to predict EC in solid wood without the infection of grain angle.

Background

The trees produce various types of wood timber for industry and society construction. One of the most valuable and popular types of wood, especially in China, is the natural durable wood with splendid colours. Natural durable wood has a character of self-preservation to survive biological decay [1, 2]. On the other hand, different wood colour, for instance, yellow and red, potentially increases the value of the wood for end use. Therefore, natural durable wood with colour has been widely studied. In the tree stem, the inner part of wood is called heartwood, and the outside of wood is recognized as sapwood. As the tree growing, cells in the inner part of sapwood begin to die and accumulate massive secondary metabolites, meanwhile, the sapwood turns into heartwood with natural durability and colour [3]. However, the traditional methods to test the wood natural durability are costly and time-consuming. It is reported that the extractives in the heartwood play an important role in the forming process of colour and natural durability [4]. Decomposition and colourlessness will occur when the extractives are removed from the durable wood [5]. Therefore, the amount of EC in heartwood has been studied as a proxy for natural durability [6].

The variation of EC in heartwood is huge and can be decreased by the genetic selection [7]. There are different ways to determine the quantity of extractives in heartwood. The traditional methods such as Soxhlet and accelerated solvent extraction (ASE) [8] which are time- and cost- consuming are not suitable for tree breeding and selection programs, which rely on the measurement of large numbers of samples. A high throughput and rapid measurement method for EC is needed.

Near infrared spectroscopy (NIR) is a non-destructive technique that is used for the analysis of the composition of chemical compounds in general [9-11]. It is applied to determine the quantity of

heartwood extractives in some tree species [12-14] and yields promising and reliable results. The NIR spectra collected from different samples, wood powder and solid, influence the performance of wood traits prediction model.

The models that are built on the different size of milled wood powder are different and perform higher accuracy than the model based on the solid wood when predicting the chemical properties in eucalyptus wood by NIR spectroscopy [15]. However, wood sample grinding is also a time-consuming step and reduces the extractive content prediction time. EC prediction from the solid wood samples is a suitable alternative way for NIR model calibration.

NIR spectra taken from the solid wood samples are influenced by many factors, such as moisture content [16] and grain angle [17]. It is claimed that the grain angle influences the EC prediction of *Eucalyptus bosistoana* with NIR spectra and this influence is able to be minimised by external parameter orthogonalization (EPO) algorithm [6]. Alternatively, this influence will be reduced by feature selection methods. One of the most important feature selection methods that can help to rid NIR calibrations of confounding effects [18-20] is called significant Multivariate Correlation (sMC) [21]. Aims to find the most important variables in NIR spectra and remove the irrelevant variables that influence the accuracy of the model prediction when predicting the target chemicals content in plant, it is a good way to conduct the method of feature selection combined with partial least squares regression (PLS). However, the important features in the NIR spectra for the grain angles and EC are little known.

T. sinensis is a native Chinese tree species that has been widely distributed in China, it has a long history of cultivation for its digestible buds in China. In addition, *T. sinensis* also has the advantages of fast growing and bright red heartwood which lead to wide use for furniture and industry. It is widely studied in many fields, including the cultivation, reproduction, biological activity of *T. sinensis*, and the physical and chemical characteristics of its wood. However, little is known about the nature durability and red colour timber. To establish a high quality breeding program for durability and red wood selection, it needs to find an alternative way to allow a fast and efficient measurement of the heartwood quality of *T. sinensis*. If NIR can be successfully used to analyse the heartwood properties without any grain angle influence, the traditional methods which are time- and cost- consuming can be replaced and consequently, it will give a lot of benefit for selection.

Hence, This study will focus on the effect of grain angle on NIR spectra obtained from *T. sinensis* cores, and study the possibility of applying NIR as a rapid and precise method to predict the extractives content from the solid core samples of *T. sinensis* without grain angle influence.

Results

PLS models with full length of NIR spectra

Table 1 shows PLS regression models for calibration and validation from the spectra with and without pre-processing constructed with EC and grain angle. Calibration model has different accuracy between EC

and grain angle. Regardless of the pre-processing methods, wood core NIR spectra combined with PLS model lead to a good result to discriminate wood longitudinal growth direction (0°) and cross section(90°). PLS regression model for EC shows lower R^2 result comparing to grain angle. The number of component of models appears to need more in grain angle than in EC. Compared to other different pre-processing methods, the PLS regression models combined with SNV + 1st derivative yield the best results with R^2_{CV} 0.81 and $RMSE_{CV}$ 1.52 for calibration and R^2_v of 0.83 and $RMSE_v$ 1.43 for validation. However, different pre-processing methods do not promote much robust model for grain angle.

Table 1 PLS regression models for calibration and validation of EC and grain angle with and without pre-treatment methods

		Calibration			Validation	
	Pre-treatment	R^2_{CV}	$RMSE_{CV}$	LVs	R^2_v	$RMSE_v$
EC	No (raw spectra)	0.75	1.69	10	0.79	1.74
	SNV	0.76	1.64	8	0.78	1.55
	1 st derivative	0.79	1.52	6	0.81	1.42
	2 nd derivative	0.80	1.61	8	0.81	1.52
	SNV+1 st derivative	0.81	1.52	7	0.83	1.43
	SNV+2 nd derivative	0.75	1.70	10	0.79	1.63
Grain angle	No (raw spectra)	0.87	11.32	14	0.91	9.85
	SNV	0.89	10.03	12	0.91	9.97
	1 st derivative	0.89	9.98	10	0.92	9.76
	2 nd derivative	0.88	10.34	10	0.90	9.99
	SNV+1 st derivative	0.90	9.75	11	0.93	9.54
	SNV+2 nd derivative	0.89	10.11	14	0.91	10.01

NIR spectra

The result shows that SNV + 1st derivative performs the highest ability for EC prediction by PLS model. Therefore, SNV + 1st derivative pre-processing method was taken for optimal wavenumbers selection. SNV+1st derivative spectra of wood discs are shown in Fig1. Although all spectra have a very similar shape, there is still huge variability in absorbance. The significant multivariate correlation of grain angle is mostly observed between 9000 and 7000 cm^{-1} , there is some overlap with SMC of EC in this region. The effect of grain angle performing on the spectra from 9000 to 7000 cm^{-1} and 5000 to 4000 cm^{-1} is stronger than the region from 7000 to 5000 cm^{-1} , especially the region around 8800, 7400, 7100 and 4200 cm^{-1} .

Fig. 2 shows the significant multivariate correlation (sMC) of EC (line dotted red) and grain angle (solid black) on PLS model for each wavenumber of the *T. sinensis* heartwood spectra. It can be clearly seen that the important wavelengths variables for EC and grain angle have some overlap region. However, some regions can be clearly distinguished between EC and grain angle, the most important region for grain angle mainly located at 8200 to 7800 cm^{-1} . The region around 6000 and 8500 cm^{-1} is highly related to EC with no grain angle influence. Therefore, the important region that the only high correlated to EC prediction (the both points in Fig. 2) was selected for PLS model calibration. The important region of the grain angle and other irrelevant variables have been removed from the NIR spectra.

PLS models with sMC selection

The PLS calibration models for EC and grain angle with these selected wavenumbers are shown in Table 2, In total, 19 wavenumbers are selected, which correspond to less than 1% of the total number of wavenumbers. With the prior selection of wavenumbers for EC, the R^2 of EC calibration is still high (0.82) with a low RMSE of 1.44 conversely. Simultaneously the R^2 for grain angle has been hugely reduced from 0.90 to 0.33,which significantly reduces the influence of grain angle on NIR spectra when calibrating for EC. The reference values versus NIR predicted values plot of the leave-one-out cross-validation for EC in the calibration sets and validation sets are displayed in Fig. 3. It shows that the samples are reasonably well distributed both in calibration and validation. With the sMC selected variables, PLS model yields higher accuracy of EC prediction without the grain angle influence.

The scores plot of PLS models applying both full length of NIR spectra and the sMC selection variables are shown in Fig. 4. It shows clearly that without the sMC selection, the grain angle has significant influence on EC. The EC based on these two groups is clearly distinguished (Fig. 4 (a)). However, improved with sMC selection, these two angle groups of the EC prediction are mixed together, the influence are successfully reduced (Fig. 4 (b)).

Table 2 PLS regression models for calibration and validation of EC and grain angle with selected variables and SNV+1st derivative

			Calibration			validation	
	Pre-treatment	Number of variables	R^2_{cv}	$RMSE_{cv}$	Ncomp	R^2_v	$RMSE_v$
EC	SNV+1 st derivative	19	0.82	1.44	7	0.84	1.35
Grain angle	SNV+1 st derivative	19	0.33	45	7	0.38	50

Mode check

The selected model was tested on the validation data. The EC prediction of PLS model using the full spectra is different between 0° and 90° angle. The EC at 90° shows higher than at 0°. The result shows that there is no statistical significant difference between the measurement of 0° and 90° grain angle direction when taking use of the NIR model with SMC selected wavenumbers to predict the EC (Fig. 5). Therefore it comes the conclusion that the grain orientation doesn't affect the assessment of extractive content on cores by NIR. In addition, during to the lower RMSE and higher R^2 of SMC model, the predicted distribution range of EC in these two of grain angles by SMC selected wavenumbers model is smaller than using the full length of spectra model.

Discussion

T. sinensis has a long history of culture for its digestible buds in China. The heartwood of *T. sinensis* is also valuable and has a huge potential furniture market [22]. To analyse the wood properties for genetic selection, a fast and efficient way to realize the wood properties is needed. NIR spectra of solid wood is recognized to be a potential method for predicting wood properties [23]. Similar to our result, we successfully make use of wood cores NIR spectra to predict the EC in the heartwood of *T. sinensis*. The influence of grain angle of wood samples on the NIR spectra when other chemicals need to be predicted has been studied for a long time. In our study, we found that the EC prediction of *T. sinensis* from PLS model was influenced by the grain angles. Supported by Li and Altaner [6] who employed NIR spectroscopy to predict the EC in *Eucalyptus bosistoana* and showed that the grain angle had significantly influence on the EC prediction model, the grain angle influence was removed after the EPO algorithm being applied, which was different from our study. Gierlinger, et al. [24] evaluated the difference of spectra of heartwood from axial and radial face to classify three species of larch. They addressed that spectra from axial faces showed less heterogeneity among larches. Schimleck, et al. [25] compared the accuracy of two different NIR models based on the spectra of radial-longitudinal and radial- transverse face to predict wood property. The result showed that radial-longitude provided a stronger calibration model than radial- transverse. Fujimoto, et al. [26] found that grain angle had an influence on the reflectance of spectra when collecting spectra from the wood surface on difference angles. The difference in model accuracy of grain angle estimation from the wood cross section and radial section can be explained by the variation of anatomical structures from the different surfaces. The exposure of parenchyma cells in radial section is higher than in cross section. Thus, the absorption bands present which related to cellulosic features. They are the main factors for mechanical properties and vary from different surfaces.

It is imperative to find out the dominant variables from multiple sources of NIR variation related to grain angle should be removed when calibrating PLS model for EC. The SMC method which is developed by Tran, et al. [27] can be efficiently used for important variable selection. SMC can provide an optimal

variables list which is the most correlated to the response. These variables with minimal false negative and false positive errors improve the predictive performance of the PLS model.

Two strong water absorbance bands exist around 7070 and 5100 cm^{-1} , which are similar to the 1st overtone of OH- bands. It is reported that the peak band approximately 6000 cm^{-1} , due to the 1st overtone of C-H stretching vibrations of methyl, methylene and ethylene groups, is mostly relevant to the extractives [28]. Some differences between 0° and 90° have been observed from band 9000 to 7000 and 5500 to 4000 cm^{-1} and are related to cellulose [26, 29-31].

The significant multivariate correlation of grain angle is most observed between 8500 and 7500 cm^{-1} , there is some overlap in this region with SMC of EC. However, NIR spectra have some high correlation with EC from region 6000 to 4000 cm^{-1} and have low correlation with grain angle. It shows no correlation with grain angle especially at ~ 6000 and 5400 cm^{-1} . The similar result is obtained by Schwanninger, et al. [28]. It is claimed that it is possible to select NIR spectra for calibration EC without grain angle influence. Hence, according to the SMC result for both EC and grain angle, the region of NIR spectra of high correlation with EC and low grain angle is selected for calibrating PLS model.

The robustness of our prediction model for EC hugely reduces the influence of grain angle, which makes it easier to measure the cores, because the grain in the cores is of uncertainty caused by the difficulty to locate the 'up and down' orientation of the tree in the core and the grain variation inherent in the tree. The model is developed in this study with a promising and reliable method for predicting EC in solid wood. Compared to grind wood samples into powder, it provides a fast and non-destructive way to save time and cost for analysing.

Conclusions

Our study demonstrates that it is possible to predict EC in heartwood of *T. sinensis* by establishing NIR PLS regression models from solid wood samples. With the prior wavenumbers selected by SMC method which reduces the infection of grain angle on NIR spectra, the result yields a promising and efficient prediction method for EC in heartwood without the impact of grain angle. Furthermore, it is not necessary to consider whether the NIR spectra measures cores or the powder of the grind wood to obtain powder spectra for prediction. NIR spectra of solid wood serves as a fast and non-destructive method for forest tree breeders, and it improves the efficiency to screen *T. sinensis* for heartwood quality with the assistance of NIR spectroscopy.

Materials And Methods

Materials

T. sinensis was planted in 2006 at Kaihua Forest Farm, Zhejiang province, P.R. China (118°20'E–129°12'N). 52 open-pollinated families were randomly block designed as 4 tree plots and repeated 10 times. The

annual average precipitation and temperature in this site are 1814 mm and 16.3°C respectively.

Sample processing

223 wood cores, with 14mm diameter, were taken from the bottom of tree trunk of 12 years old *T. sinensis*. Cores were labelled directly on the surface and placed into a paper bag. All samples were being air-dried for a month until a stable moisture condition was obtained. After being air-dried, the longitudinal growth direction (0°) and cross section (90°) of each core sample were marked. The surface of 0° and 90° were then sanded by a P100 medium-sized grit sandpaper to obtain a consistent surface for NIR spectra collection.

NIR spectral measurements

NIR spectra from cores were taken at room temperature with a fibre optics probe (Antaris II System, Thermo Electron Company, USA) at wavelength from 9000 to 4000 cm^{-1} at 10 cm^{-1} resolution. Each NIR spectrum was taken at regular intervals (5 mm) from pith to bark in heartwood along the 0° and 90° surface of cores and calculated the average weight. Average 64 times scanning of each spectrum leaded to one final spectrum.

EC extraction

Each core was cut into small chips with a chisel and milled into fine powder with a 2-mm screen. The wood powder sample was oven dried at 60°C to obtain a stable moisture content. All cores samples were prepared for extraction after the NIR spectra collection. The accelerated solvent extraction (ASE) was processed supported by the thermo accelerated solvent extractor 350 (Thermo Fisher Scientific, Bellefonte, PA, USA) with ethanol. The methods were similar to Li and Altaner [6] . 4g of wood powder was placed into a stainless steel cells and the setup extraction process was as following: static time 15 mins, temperature 70°, 100% rinse volume and 2 extraction cycles. The extractive solutions of samples were collected into a dry aluminium foil tray with known mass and placed in the fume cupboard overnight for the ethanol to evaporate. Subsequently the extracts were dried in an oven overnight at 105 °C to remove moisture. The mass of the extract was determined and the extractives content was calculated on a dry mass basis. EC for the samples was ranging between 1.23 % and 16.49% with an average of 8.86%.

NIR spectra processing

To find out whether the grain angle has effect on the NIR spectra for EC prediction in *T. sinensis* or not. The optimal range of the spectrum for accurate calibration was investigated. PLS regression was used to

perform grain angle classification analysis and to predict EC. The data from the samples was divided into two data set by Kennard-Stone sampling with Euclidean distance [32], including 200 selected samples as calibration data and the remaining 37 as validation data set for PLS model calibration and validation. Different spectra pre-processing was applied on the NIR data sets before model calibration to character the best suitable pre-processing method, which includes standard normal variation (SNV), 1st and 2nd derivative of Savitzky-Golay algorithm with a 2 order polynomial and 15 window sizes. A filter method [33] which is called significant multivariate correlation (sMC) was carried out to find out the most important variable for grain angle and EC respectively and to eliminate the unimportant variables and develop a more reliable and robust model for EC prediction. The coefficient of determination (R^2) and root-mean-square error (RMSE) derived from both the calibration (R^2_{CV} and $RMSE_{CV}$) and validation (R^2_V and $RMSE_V$) were implemented to track the model performance. Data analysis was conducted in R software (version 3.1.2) [34]. The pls package [35] was used for PLS and sMC-PLS model performing and the plsVarSel [33] for sMC variables selection. The prospectr package [36] was used for NIR spectra manipulation and Kennard-Stone sampling, and the ggplot2 package [37] for visualization plot.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data and material

Not applicable.

Competing interests

The authors declare that there is no conflict of interest.

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Authors' contributions

Yanjie Li designed the study, conducted the experiment, analysed the data and wrote the manuscript. Xin Dong and Yang Sun conducted lab experiments, Jun Liu and Jingmin Jiang supervised the experiments at all stages and reviewed the manuscript. All authors have read and approved the final manuscript.

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Authors' information

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Figures

Figure 1

SNV+1st derivative absorbance spectra of average 0 and 90 degree between 9000cm-1 and 4000cm-1 in cores

Figure 2

The influences of grain angle and EC on NIR spectra of *T. sinensis*. In this graphs, sMC_angle: black solid line; sMC_EC: red dash line; SNV+1st: green dote line; Optimum wavenumbers selected: Blue area.

Figure 3

The best calibration model for EC with selected wavenumbers without influence of grain angle with the measured versus predicted values in the (left) calibration and (right) validation sets.

Figure 4

the scores plot of PLS model for EC prediction based on the full length of NIR spectra and the sMC optimal selected spectra variables.

Figure 5
predicted EC on *T. sinensis* validation cores samples dependent on grain angle with and without sMC variables selection.