

WOOD MOISTURE CONTENT DETERMINATION BY HANDHELD NEAR-IR REFLECTANCE SPECTROMETER

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Abstract. Rapid, accurate determination of wood moisture content is paramount for the wood industry, infrastructure maintenance, studies of plant physiology, and forest management. Near-IR reflectance spectroscopy (NIRS) is a widely used nondestructive technique for analyzing the properties of materials, including MC. Small, portable, handheld NIR spectrometers represent an emerging technology with strong potential for rapidly, affordably estimating materials properties. Here, we used a SCiO™ miniature handheld NIR spectrometer and a partial least squares regression model to predict wood MC. The model was developed using spectra (740-1070 nm) collected from increment borer wood samples from 41 representative softwood and hardwood trees, calibrated against gravimetric wood MC determined by oven-drying. The calibration and prediction datasets contained 2/3rd and 1/3rd of all data, respectively. We explored the effects of different spectral preprocessing algorithms (ie first and second-order derivatives and standard normal variate transformations) on model performance. First-order derivative spectra with five latent variables yielded the most robust model (R^2 : 0.72, RMSEP: 0.32, the ratio of performance to deviation: 2.2). Broadly, we demonstrated that relatively low-cost miniature handheld NIR spectrometers such as the SCiO™ can rapidly estimate percent MC in the wood of various species.

Keywords: Biometry, moisture content, near-IR spectroscopy, rapid measurement, wood.

INTRODUCTION

Moisture content is an important wood quality variable (Leblon et al 2013), influencing its weight, volume, elasticity, tensile and compression strength, milling properties, and thermal yield during combustion (Mitchell 1961). Determining MC gravimetrically (by weighing a sample before and after oven-drying) is time-consuming. It requires destructive sampling, while passive methods such as Fourier transform IR spectroscopy and X-ray tomography require bulky, costly, and specialized laboratory equipment with limited portability (Leblon et al 2013; Pu et al 2021). Compact, low-cost (~USD 800 in 2024), portable handheld near-IR (NIR) spectrometers represent an emerging

technology for affordable, rapid determination of MC in wood in the field, mill, or laboratory.

NIR spectroscopy measures light (400-2500 nm) reflected from a material surface to reveal the chemical bonds associated with various functional groups (eg OH, CH, NH) within the material (Ma et al 2019). The electrons in the O-H bonds of moisture (water) interact specifically with photons corresponding to the following NIR bands: 760, 970, 1190, 1450, and 1940 nm. Broadband or narrow-band spectra can be calibrated against gravimetrically determined MC in reference samples using a multidimensional regression model, which can be used subsequently to predict the MC in samples with similar physicochemical

properties (Kelley et al 2004; Via 2004; Leblon et al 2013; Sundaram et al 2015; Liang et al 2019). In addition to benchtop NIR spectroscopy instruments, many miniature NIR spectrometers have been developed (Li et al 2018; Wiedemair et al 2019; Cazzaniga et al 2022). Compared with the broad spectral range (400-2500 nm) and higher resolution data acquired by benchtop NIR spectrometers, these miniature devices typically acquire narrower band spectra with lower resolution (Pillonel et al 2007; Digman et al 2021; Nkouaya Mbanjo et al 2022; Cazzaniga et al 2022). One example is the handheld SCiO™ spectrometer (Consumer Physics Inc., Tel Aviv, Israel) that can acquire a spectrum ranging from 740 to 1070 nm (wavelength resolution $<10\text{ cm}^{-1}$, sampling frequency: 1 nm). Multiple studies have demonstrated the feasibility of using miniature NIR spectrometers to determine physiochemical properties, such as the proportion of solids, moisture, sugar, and protein in agricultural commodities (eg cheese, hay, corn, apple, kiwifruit, and feijoa [Li et al 2018; Digman et al 2021; Cherney et al 2023]).

Collecting NIR spectral data in the field can be challenging due to variable and suboptimal environmental conditions (eg temperature, humidity), which can potentially decrease measurement precision, accuracy, and resolution. To maximize reliability, the devices should be trained (calibrated) to generate accurate predictions from relatively wide NIR spectral bands acquired under the anticipated range of operating environmental conditions. Because of methodological innovations in machine learning algorithms, increasing affordability and accessibility of computational processing, and affordable data storage, machine learning has become a valuable method to process complex data rapidly and accurately on a large scale, with minimal human intervention. Spectral pretreatments, such as standard normal variates (SNV), first-order derivatives (FD), and second-order derivatives (SD) can increase the reliability of quantitative measurements predicted from NIR spectra and be readily performed on recent versions of personal computing devices such as smartphones. SNV reduces the multiplicative interference present in spectral data (Cazzaniga

et al 2022). FD enhances the peaks of the spectral data or reduces the effect of additive baselines, and SD can reduce the effect of multiplicative baseline scattering (Ferrara et al 2022b).

Partial least squares (PLS) regression is a common and effective machine learning algorithm for generating predictive models by calibrating pre-processed NIR spectra against quantitative measurements determined by a secondary method (Li et al 2018; Wiedemair et al 2019; Cazzaniga et al 2022; Ferrara et al 2022a, b; Nkouaya Mbanjo et al 2022). PLS regression utilizes a combination of principal component analysis and multivariate linear regression models involving two sets of data: calibration (training) data and prediction data (Geladi and Kowalski 1986). Calibration model fit and predictive accuracy are iteratively optimized by cross-validation using different subsets of the data (eg 2/3rd of the dataset for calibration and 1/3rd of the dataset for assessing prediction quality). The data quality metrics, namely coefficient of determination (R^2), root mean square error (RMSE), and the ratio of performance to deviation (RPD) are internal validation parameters used to assess calibration model performance (Cazzaniga et al 2022; Ferrara et al 2022a, b; Haruna et al 2022). R^2 (range 0-1) is a variant of the R^2 adapted to n -dimensional space, and as with its 2-dimensional counterpart, a value closer to unity indicates a better calibration model fit. RMSE quantifies the calibration precision, representing the standard deviation of calibration errors. RPD measures the predictive power and accuracy of the calibration model, with higher RPD values (generally >3) being desirable (Rubert-Nason et al 2013; Cazzaniga et al 2022; Ferrara et al 2022a, b; Haruna et al 2022).

In this study, we calibrated and validated a model for predicting the MC of green wood in live forest trees using a low-cost, compact, handheld NIR spectrometer. We hypothesized that a predictive model developed using machine learning would enable the determination of MC in wood from the relatively low-resolution, narrow-band NIR spectra provided by this type of instrument. The influence of various spectral preprocessing combinations on the power of PLS regression for MC

prediction was compared in terms of R^2 , RMSE, and RPD.

MATERIAL AND METHODS

Study Site and Data Collection Tools

Wood increment cores (7-10 cm long) for model development and testing were collected from hardwood and softwood trees of merchantable size (41 total, diameter at breast height circa 10-20 cm, core length: 7-10 cm) within the Fournier Biological Park at the University of Maine at Fort Kent (47.246910N, -68.592626W). We developed a single calibration model for estimating MC in wood of the following taxa that are commonly found in northern mixed forests of North America: Poplar (*Populus* spp.), Balsam fir (*Abies balsamea*), Birch (*Betula* spp.), Black ash (*Fraxinus nigra*), Spruce (*Picea* spp.), Cedar (*Thuja occidentalis*), Red pine (*Pinus resinosa*), Pin cherry (*Prunus pensylvanica*), and Maple (*Acer* spp.) (Sibley 2009). The numbers of each species represented in the calibration set represented the approximately uniform abundances of these different species in the sampling site, permitting the development of a single calibration model optimized for determining wood MC in northern mixed forests.

Within 10 min of collection, cores were scanned at a single location near the center along the radial edge with a handheld NIR spectrometer (SCiO™, v 1.2; Consumer Physics Inc.), and the data were stored in the Cloud provided by the vendor. Core samples were promptly placed inside labeled paper envelopes, bundled together, and transported inside plastic bags within a cooler box to prevent moisture loss.

Spectral Data Collection and Mathematical Treatment

Spectral acquisition. Reflectance spectra (six scans per sample spanning 740-1070 nm) were collected for each of the wood cores, by scanning against a white background (Fig 1). The wood samples were weighed when wet, dried in an oven to constant weight at 60°C, and weighed again to determine gravimetric wood MC. Wood

MC was calculated and reported as a percentage of dry wood weight.

Spectral preprocessing. We evaluated the effects of using broadband (740-1070 nm) and narrow-band spectra (760 and 950-970 nm) and the following spectral pretreatments on PLS model performance: SNV, FD, and SD. These transformations were tested alone and in combinations to evaluate their impacts on the prediction power and identify the combination with optimal accuracy. For optimizing the selection of preprocessing transformations (Fig 1), we followed a similar approach to Ferrara et al (2022a, b).

PLS Regression Models

We subjected spectral data under various preprocessing combinations to PLS regression to create and select the optimal model for predicting wood MC. The dependent variable was the gravimetric MC (% w/w) of the wood samples and the independent variable was the reflectance of light across the entire 740-1070 nm band. The data set was divided into calibration (training) and validation (test) subsets using the Kennard-Stone sampling method (Kennard and Stone 1969). Calibration data comprised two-thirds of the total samples and prediction data comprised one-third of the total samples.

Spectral preprocessing and PLS regression were computed using Origin Pro (version 2023b; OriginLab Corporation, Northampton, MA). The RPD was calculated using the method of Pillonel et al (2007). The calibration model was cross-validated using 10-fold cross-validation. Following this method, once a calibration model was built based on a subset of the data (calibration dataset), the remaining subset (prediction dataset) was subjected to the model for prediction of MC, and the model was iteratively refined. In this way, the performance of the calibration model was evaluated by the optimal number of latent variables, R^2 , RMSE%, and RPD.

RESULTS

Wood spectra varied concerning MC, particularly in the moisture-absorbing bands (760 and

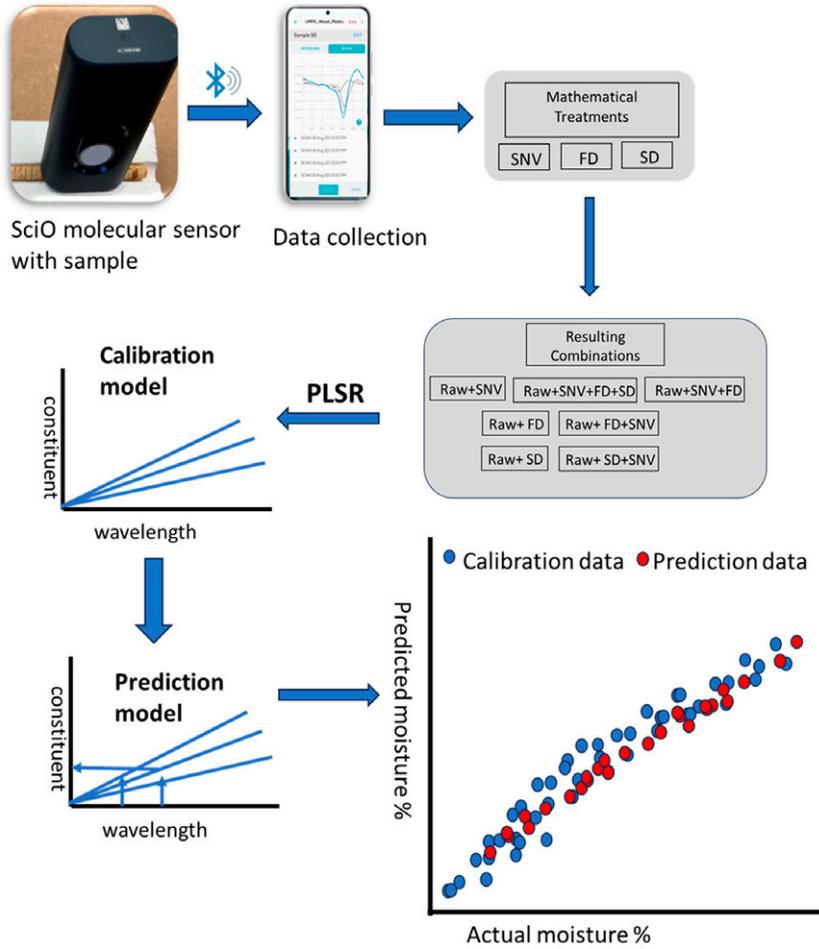


Figure 1. Process flow for data acquisition, calibration model development, and validation for determining wood MC by narrow band near-IR spectrometry showing a theoretical plot of predicted vs actual MC. FD, first-order derivative; SD, second-order derivative; SNV, standard normal variate; PLSR, partial least squares regression.

950-970 nm), and spectral preprocessing influenced the magnitude of features associated with variations in MC (Fig 2). The relative standard deviation (RSD) of the six NIR spectra scanned for each tree sample, averaged across all 41 samples, varied by wavelength from 0.043 to 0.074 (as a proportion of average spectral amplitude at a given wavelength). Within any particular sample, the RSD ranged from 0.0003 to 0.254 (Fig S1). Strategic selection of preprocessing treatments (ie normalization SNV, FD, and SD) was essential to maximizing spectral differences relating to MC

(Fig 2) and the predictive power of the resultant calibration (Table 1).

Selection of broadband vs narrow-band spectra (focused on moisture-absorbing wavelengths) had minimal impact on PLSR calibration *model fit* (evidenced by $R^2(C)$ and $RMSE(C)$); but the *predictive power* of PLSR models based on broadband spectra was superior (evidenced by $R^2(P)$, $RMSE(P)$, and RPD) (Fig 3; Fig S2). The choice of spectral preprocessing methods also substantially influenced the performance of PLSR

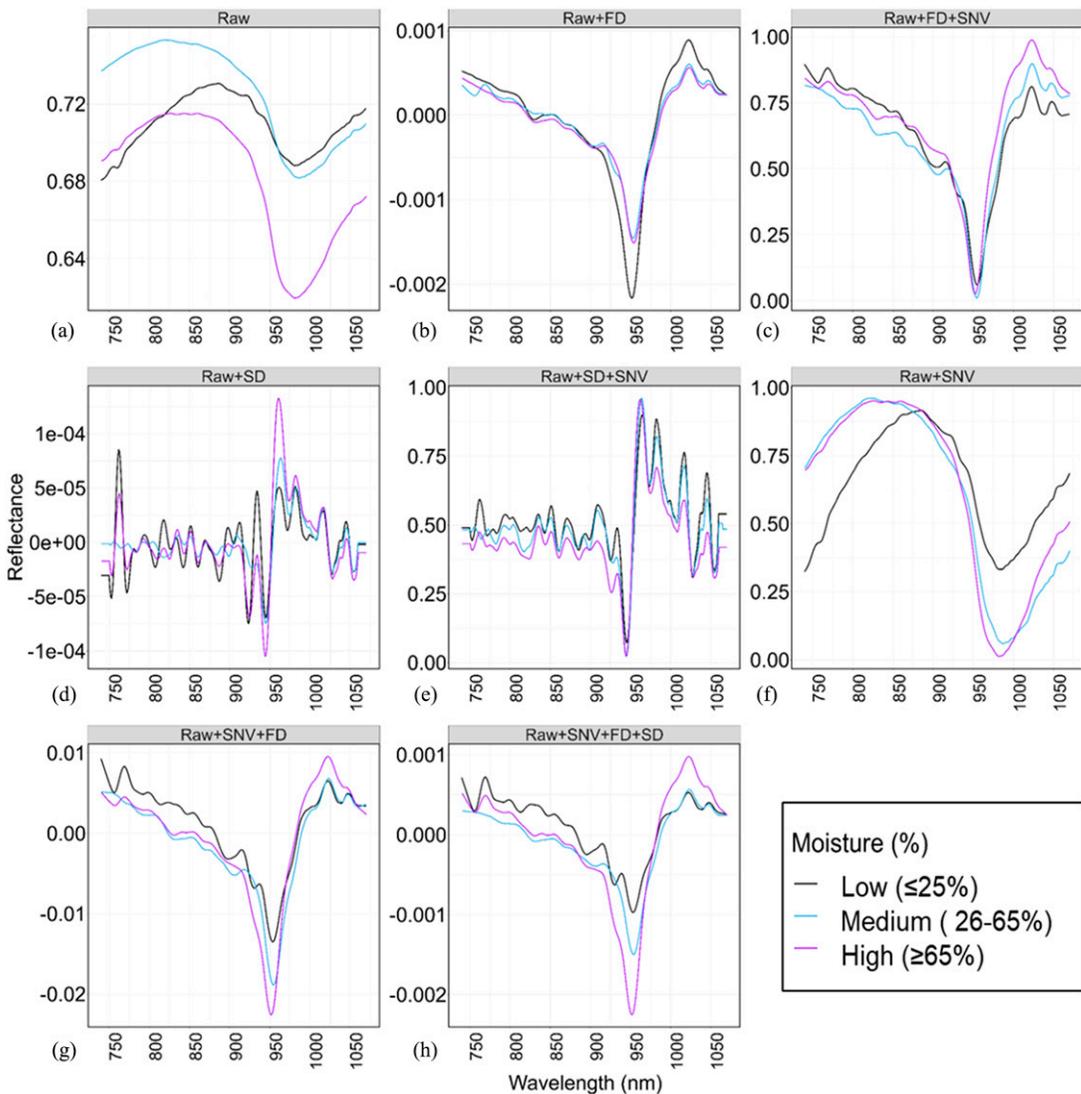


Figure 2. Influence of spectral preprocessing on the visual distinction between low ($\leq 25\%$), medium (26-65%), and high ($\geq 65\%$) wood moisture levels. (a) Raw reflectance data for reference; (b-h) effects of different spectral preprocessing method combinations on features associated with differences in wood MC. FD, first-order derivative; SD, second-order derivative; SNV, standard normal variate.

calibration models. Collectively, $R^2(C)$, $R^2(P)$, RMSE(C), RMSE(P), RPD (Table 1), and the correspondence between predicted and actual (secondary) validation measurements of wood MC (Fig 3) revealed that the optimal calibration was obtained with first-derivative pretreatment of broadband spectra (Table 1). Other pretreatment permutations involving first derivative and SNV transformations also produced potentially useable,

albeit less accurate calibrations. Some calibration models fit the training dataset well (ie spectra with SNV+FD pretreatment), but predicted MC less reliably (RPD: 2.0).

DISCUSSION

Our study reveals that miniature, narrow bandwidth NIR spectrometers such as the SCiO™ can

Table 1. Quality criteria for partial least squares regression models fitted to reference wood MC and broadband spectra under different spectral pretreatments.

Spectral preprocessing combination	LV	$R^2(C)$	RMSE(C)	$R^2(P)$	RMSE(P)	RPD
Raw, FD	5	0.86	0.60	0.72	0.32	2.20
Raw, FD, SNV	7	0.80	0.76	0.72	0.68	1.03
Raw, SD	7	0.97	0.36	0.74	0.39	1.80
Raw, SD, SNV	1	0.48	0.85	0.55	0.32	2.19
Raw, SNV	8	0.80	0.75	0.80	0.48	1.46
Raw, SNV, FD	8	0.88	0.74	0.58	0.35	2.00
Raw, SNV, FD, SD	Calculation was terminated due to model overfitting					

LV, latent variables; R^2 , coefficient of determination; RMSE(C), root mean square error of calibration; RMSE(P), root mean square error of prediction; RPD, ratio of performance to deviation; FD, first-order derivative; SD, second-order derivative; SNV, standard normal variate.

provide rapid and cost-effective estimates of MC in the wood of northern temperate forest trees. Our best calibration against gravimetrically determined reference values, obtained by PLS regression with first-derivative broadband spectra as is common in quantitative NIR (Vibhute et al 2018), met validation criteria (R^2_C : 0.86, R^2_P : 0.72, RMSE: 0.32, and RPD: 2.2) that are generally

regarded as acceptable for meaningful predictions ($R^2 > 0.70$, RMSE: small [Rubert-Nason et al 2013; Li et al 2018]). Nevertheless, an RPD of 2.2 was less than the preferred threshold of 3.0 and indicated that predictions were of limited precision. Relative to larger, more costly spectrometers such as the Foss NIRSystem 5000 (1100–2498 nm bandwidth) (Yang et al 2024), spectra

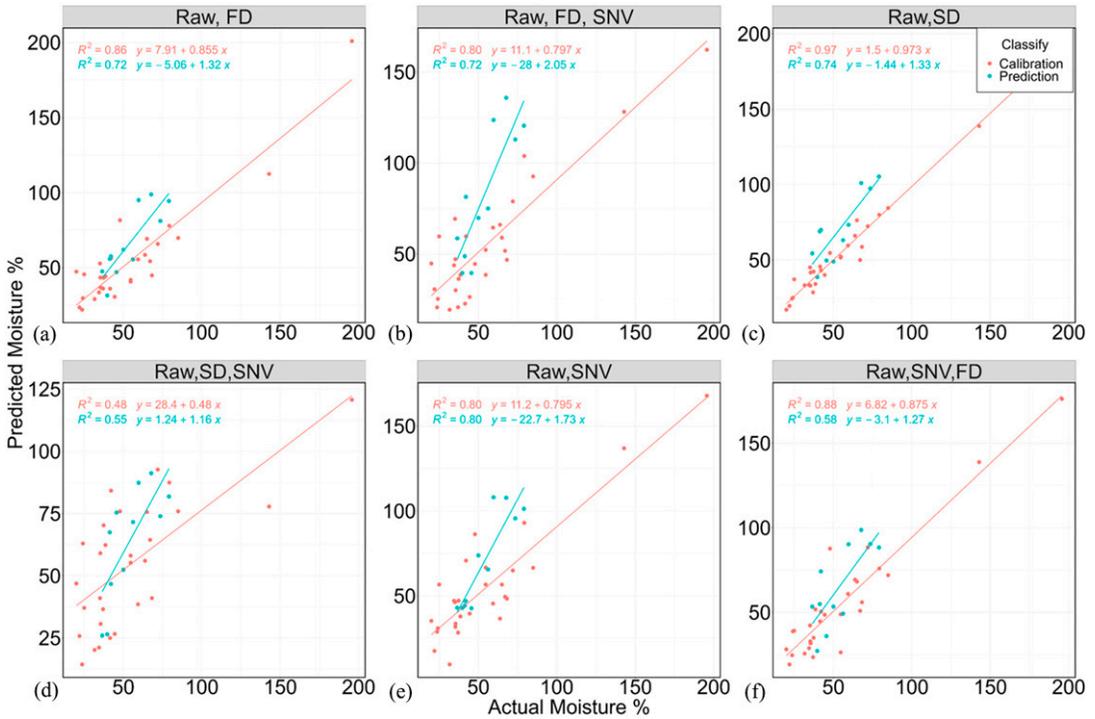


Figure 3. Predicted vs actual wood MC by partial least square regression models fitted with spectra subjected to different preprocessing treatments. (a-f) Effects of different spectral preprocessing method combinations on wood moisture prediction. FD, first-order derivative; SD, second-order derivative; SNV, standard normal variate.

acquired with the SCiO™ were of comparatively lower resolution. The quality of the PLS model fit for moisture determination with the miniature NIR device (R^2 : 0.8) was also correspondingly lower than that of the benchtop NIR sensor (R^2 : 0.92) (Kaur et al 2017).

The selection of spectral pretreatments is vital to optimizing the predictive power of the PLS model, as evidenced by large variations in the PLS model predictive power in response to the different pretreatment combinations that we explored (Table 1). Selecting a specific preprocessing method is a trial-error process and cannot be addressed prescriptively (Agelet and Hurburgh 2010). Optimizing model fit based on different permutations of common pretreatments (ie SNV, FD, SD) adjusts the baseline and scales the spectra to enhance the weighting of moisture effects (SNV), delineate moisture-related peaks (FD), and reveal more nuanced spectral qualities associated with MC (SD). It is essential to optimize combinations of spectral pretreatments for both model fitting and model predictions because some combinations may produce a strong model fit but less reliable model predictions (as we observed with SD+SNV spectra), and to avoid too many spectral pretreatments as they can lead to model overfitting (ie SNV+FD+SD).

Although the predictive power of miniature NIR spectrometers is limited by hardware characteristics such as narrower bandwidths and lower sensor resolutions compared with larger benchtop devices, it may be possible to increase their predictive power by strategic calibration model selection and diversification of training data sets. While PLS is a common approach to instrument calibration (Li et al 2018; Wiedemair et al 2019; Cazzaniga et al 2022; Ferrara et al 2022b; Nkouaya Mbanjo et al 2022), alternatives such as modified PLS (Rubert-Nason et al 2013), principal component regression (Vigneau et al 1997), and neural network analysis (Wu et al 1996) have occasionally been used and merit further exploration. While developing calibrations for moisture determination using only the two specific, strong spectral maxima for water (760 and 950-970 nm [Kasim et al 2021]) within the SCiO™ spectrometer's operating

range (740-1070 nm) would be desirable to increase method specificity and decrease potentially interfering covariances, this action resulted in calibrations with less predictive power. We speculate that the detrimental effect of restricting our spectra to specific narrow bands may be a consequence of insufficient spectral data—attributed to the lower resolution of our instrument.

Multiple authors have examined how the diversity of training sample sets impacts the quality of calibration model fits and predictions. The general trend for PLS calibrations is that prediction power decreases as the diversity of the training sample set increases. For example, the inclusion of a broader range of tree species and ages is associated with lower R^2 values in some calibrations (Schimleck et al 2018). In the case of the SCiO™, Ma et al (2019) compared the effects of various permutations of spectral preprocessing and regression approaches (eg PLS discriminant analysis, interval PLS, and multiple linear regression with forward and backward selection), and found that the use of the instrument's full bandwidth (740-1070 nm) and PLS regression maximized predictive power for casein (R^2 : 0.45-0.56, RMSE: 1.28-1.42, RPD: 1.4-1.5) and total protein (R^2 : 0.7-0.77, RMSE: 0.53-0.62, RPD: 1.8-2.1), but that predictive power (RPD) was less than the desired 3.0. Because factors such as spectral band selection, preprocessing, plant species, plant age, and sample set size can impact the accuracy of quantitative NIR predictions, it is likely possible to obtain more accurate estimations of wood MC with miniature NIR spectrometers by using a larger training dataset and a calibration routine that statistically accounts for these different factors. Specifically, we suggest that our calibration could be improved by using a larger sample set and a modeling algorithm that incorporates tree taxon and classification of wood samples by age and position within the tree (sapwood/heartwood).

CONCLUSION

Miniature NIR spectrometers with limited bandwidth (ie 740-1040 nm), such as the SCiO™, can provide rapid, cost-effective estimates of wood

MC in field environments when calibrated against gravimetrically determined reference values by PLS regression. However, tools like the SCiO™ appear to be less accurate, presumably due to their lower resolution compared with larger, costlier benchtop and backpack-type NIR spectrometers. Selection of spectral preprocessing routines is key, with our best-performing calibration (R^2 : 0.72, RMSEP: 0.32, RPD: 2.2) obtained using first derivatives of spectra. Further studies should aim to improve the predictive power of these miniature instruments, by expansion of training datasets to include a greater diversity of tree species, ages, and sampling locations.

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COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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