Near Infrared Spectroscopy (NIRS) as a Tool for Effective Classification of Wood

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Abstract

Wood from different tree species is commonly similar in visual appearance but still have considerable differences in machining and wood properties. Even heartwood and sapwood from the same tree species may be difficult to separate visually, but the wood properties important for the quality of the final products may differ. Hence, within the forest products industry there is a great need to non-destructively evaluate wood quality prior to and during manufacturing in order to ensure effective allocation of raw material, and to obtain consistent and well defined quality of the end products. Near infrared spectroscopy is a promising technique because it requires minimal, if any, sample preparation and provides results rapidly, even when used on intact, opaque biological samples.

In this paper we use near infrared spectroscopy combined with multivariate statistical analyses for classification of wood types. Case I considers heartwood and sapwood from Scots pine. On freshly cut wood heartwood and sapwood are visually similar, but the wood properties differ. Case II considers wood from tree different species of spruce, Norway spruce, Sitka spruce and Lutz spruce. The species have differences mechanical and machining properties.

NIR spectra were recorded directly on solid wood surfaces. The multivariate statistical analyses were based on partial least squares methodology and resulted in successful classification of wood types in both cases. All models were validated using test set validation. In both cases the result showed that near infrared spectroscopy and multivariate statistics can be used to develop well-performing prediction models for classification of visually similar wood types.

Keywords: Near Infrared Spectroscopy, classification, wood properties, multivariate statistics, validation, Scots pine, Norway spruce, Sitka spruce, Lutz spruce, partial least squares

Introduction

Characterisation and quantification of many wood properties that are of significance for the quality of the end-products are often time consuming and require destructive analyses. According to Pellerin and Ross (2002) visual inspection is one of the most frequently used non-destructive techniques in the forest product industry. The method has obvious shortcomings when important wood properties such as durability, bending strength, bending stiffness and machining properties differ even though the wood types have similar visual appearance.

A requirement for techniques used in industrial applications is that results are produced non-destructively and fast, so that the speed of the production line is not affected. Manufacturers of wood products cover a broad range of technological levels with a correspondingly broad range of non-destructive evaluation methods developed through research.

NIR spectroscopy requires minimal sample preparation and provides results rapidly, even when used on intact, opaque biological samples. Low absorptivity of water makes the NIR region suitable for analyses of samples containing water (Osborne, *et al.* 1993). The NIR spectrum extends from 780 to 2500 nm, and is created by absorption corresponding to overtones and combinations of fundamental vibrational transitions in the infrared region mainly involving C-H, O-H or N-H functional groups. The spectrum contains chemical and physical information about a sample. Various compounds in biological materials have overlapping peaks in the spectra. This implies that there is strong correlation between variables in the X-matrix which emphasises the need for multivariate statistical methods to enable interpretation of the spectra. NIR analysis relies on developing a calibration model that relates the NIR spectra of a large number of samples to the corresponding values of the response variable, measured by a reference method. The calibration model is then used to predict new samples based on their NIR spectra (Shenk, *et al.* 2001).

NIR spectroscopy is a method that has yielded promising results when used to classify various types of wood. Brunner *et al*.(1996) used NIR spectroscopy to differentiate wood from 12 tree species, mainly tropicals. Schimleck *et al*. (1996) used NIR spectroscopy and PCA for eucalypt wood classification. Borga *et al*. (1992) found that NIR spectroscopy can be used to classify milled samples from wet-stored timber of Scots pine (*Pinus silvestris* (L.)) into heartwood and sapwood. Results have also been presented indicating that NIR spectroscopy may be used to differentiate between wood samples of the same species, but from different origins (Gierlinger, *et al.* 2004). For a comprehensive overview of applications of NIR spectroscopy in the forest products industry it is referred to (So, *et al.* 2004).

In this paper two case studies are presented.

In case I we use NIRS to differentiate between dried heartwood and sapwood of Scots pine. While the heartwood of Scots pine is regarded as moderately durable and can attain

a long service life in above ground conditions, the sapwood can deteriorate rapidly when exposed to risk of decay. Solid wood products of Scots pine commonly consist of a mix of heartwood and sapwood. A board consisting of wood with considerable variation in decay resistance is obviously undesirable from a durability point of view. The more durable heartwood can, if separated from sapwood during wood processing, be beneficially utilised for products where risk of decay is a concern, e.g. external claddings, decks and window frames. It is often difficult to classify heartwood and sapwood on dried and recently machined wood (Fig. 1), or if the wood specimen consists of solely heartwood or solely sapwood.

In case II we use NIRS to differentiate between dried wood from Norway spruce (*Picea abies* (L.) H. Karst), Sitka spruce (*Picea sitchensis* (Bong.) Carrière) and Lutz spruce (*Picea* × *lutzii* Little). At present the species occur in plantations in the western and northern part of Norway. As they all prosper in the moist climate they will eventually be found also in mixed stands. The three species have different mechanical and machining properties, and should therefore be treated separately in wood processing as well as for final products. Sandland and Eikenes (1996) investigated different aspects of lumber manufacturing of Sitka spruce grown in Norway. They found that the feeding speed had to be reduced to half the normal speed used for resawing Norway spruce because the knots found in Sitka spruce are harder and have higher density. Although not investigated, it is a reasonable assumption that Lutz spruce has properties that differ from Norway spruce and Sitka spruce. For the final product, such as surfaced wood, differentiation of the three tree species can be very difficult because the wood types have similar visual appearance (Fig. 1).

Figure 1. Wood with similar visual appearance. To the left, heartwood and sapwood of Scots pine (Case I). To the right sawnwood of Sitka spruce, Lutz spruce and Norway spruce (Case II).

Material and methods

Case I – Scots pine

Material

The wood specimens were collected from six mature stands of Scots pine in the southern part of Norway. Three 200 m^2 circular sample plots were evenly distributed in each stand. Within each sample plot the trees were sorted based on their diameter at breast height, and divided in three groups each containing an equal number of trees. One tree was thereafter randomly sampled from each of the three groups within each plot. In total, 9 trees from each stand were sampled. Stem discs of sound wood were cut at 20% of tree height from each sampled tree. From each stem disc a wood block was cut from bark to pith along the radial direction of the wood. The blocks were oven-dried at 35˚C for 48 h and acclimatized in laboratory for approximately one month.

NIRS

The radial surfaces of the wood blocks were re-sawn immediately prior to NIR measurements, thereby attaining fresh surfaces where heartwood and sapwood had similar visual appearance (Fig. 1). NIR spectra were recorded directly on the radial wood surface, and wherever possible from the inner heartwood (10 mm outside the pith), the outer heartwood (avoiding the two annual rings closest to the heartwood/sapwood transition zone) and from the sapwood. In all, 159 samples were available, 54 from the inner heartwood, 53 from the outer heartwood and 52 from the sapwood. As the inner and the outer heartwood have similar wood properties, the objective of this study is to identify sapwood from heartwood using NIRS. Scanning of spectra was performed in reflectance mode, in the 400-2500 nm range (visual and NIR), in 2 nm steps, by a NIRSystems 6500 spectrophotometer with a hand held remote reflectance fibre-bundle optic probe (NIRSystems Inc, Silver Spring, MD, USA). For each measurement 32 scans were collected and averaged.

Case II – Three spruce species

Material

Sawnwood samples were produced from Norway spruce, Sitka spruce, and Lutz spruce originating from seven stands in the northern part of Norway. Four trees were collected from each stand, and a short log section from the lower part of each trunk (1.5–2.5 m above the base) was used to prepare small clear specimens (20 × 20-mm cross-sections parallel to the orthogonal planes of the wood matrix). Three specimens were produced from each tree, giving a sample of 12 specimens from each stand except for one stand where only 11 specimens were available.

NIRS

NIR spectra were collected on one of the cross-sectional faces of each of the 83 air dry wood specimens. The cross-sectional faces were prepared by circular sawing. There were no visible colour differences between wood from the three different tree species (Fig. 1). Scanning of spectra was performed in reflectance mode, in the 700 nm –2500 nm range, in 0.35-nm steps, by a PerkinElmer Spectrum One NTS system equipped with a Near Infrared Reflectance Accessory (NIRA) package. The specimens were placed directly on the circular sapphire window on top of the Near Infrared Reflectance Accessory. The diameter of the window was 10 mm. For each spectrum 25 scans were collected and averaged. Before analyses the wavelength variables were reduced (averaged) by a factor of 6. A complete description of the material and methods for Case II is presented in Flæte, *et al.*(2006).

Statistical analysis

In both cases the reflectance data was expressed as apparent absorbance (log 1/reflectance). The spectral data were centred and standardised before analysis. To correct for baseline shifts, the data were transformed to first derivatives in both cases.

The data were analysed using Partial Least Squares (PLS) Regression models. This is a linear modelling technique that compresses the spectral data and projects them on to partial least squares components. The PLS components are extracted so that the covariance to the dependent variable is maximised (Martens and Næs 1989). In addition, the PLS components are mutually orthogonal, thus avoiding the problems often encountered when there are high degrees of correlation among the variables in the X-matrix. In the PLS 2 method two or more dependent variables are modelled simultaneously. Compared to traditional statistical modelling based on least squares estimation, independent variables in the X-matrix is not a requirement for these methods, which can also handle situations where the number of variables far exceeds the number of samples, which is typical for modelling with NIR data.

PLS Discriminant Analysis (PLS-DA) involves developing a conventional partial least squares regression model, but instead of a continuous variable the response variable is a binary variable. If a variable takes the value of 1, the specimen in question is a member of that group, and consequently if a variable takes the value of 0, the specimen in question is not a member of that group. The fit of each observation is evaluated against the measured value for the same observation. The fitted value for the class indicator Y-variable is used to assign the calibrated observation to a group:

- $Y_{fit} > 0.5$ means “member”
- $Y_{fit} < 0.5$ means “non-member”

When creating models with two or more binary variables the model is referred to as PLS2-DA models. In situations where the fitted response exceeds 0.5 for more than one binary variable, the wood specimen is assigned to the group for which the model had the highest fitted response.

All statistical analyses were performed in the Unscrambler® from Camo Software AS.

Model validation

Model validation is crucial when developing prediction models, particularly in NIR spectroscopy. Reliable validation will reduce the risk of modelling variation in the spectra that are caused by random noise.

Both cases were validated using test set validation by splitting the data into a calibration set and a test set. For both cases, the specimens were assigned to a calibration and validation set based on their origin (stand), instead of splitting the data randomly or systematically. This is a conservative approach, as it is reasonable to assume that trees from the same origin are somewhat correlated with respect to wood properties. By including all specimens from one stand in the test set there is no information available in the model calibration that can be used to model the properties resulting from trees originating from the same stand.

The classification performance of the models was evaluated by calculating the proportion of specimens from the test set that was correctly classified. The models should also preferably fit each wood specimen into the correct group in the calibration step.

Case I consist of 159 wood specimens. Wood specimens from four stands were used for model calibration, while the two remaining stands were used as a test set for model validation. In the test set, there were 18 specimens of sapwood and 36 specimens of heartwood.

Case II consisted of 83 samples from 7 different stands. The calibration set consisted of the wood specimens from four of the stands (47 specimens) while the validation set consisted of 36 wood specimens (12 specimens of each species) from the tree remaining stands.

Results

Case I

When analysing the data from Scots pine – wavelength variables from 800 nm to 2250 nm were used in the analysis. Variables from 2250 nm to 2500 nm were removed due to high levels of noise, caused by the fibre optics. The resulting PLS-DA model was calibrated with five PLS components. In the model calibration, all specimens (n = 105) were fitted to the correct tree species.

Two specimens from the validation set (n = 54) were incorrectly classified. One specimen from the outer heartwood was classified as sapwood, and one sapwood specimen was classified as heartwood. Hence the overall classification performance is 96,3%, while for heartwood and sapwood the classification performances are 97,2% and 94,4% respectively. The two incorrectly classified samples both originated from the same stand. This stand was older (231 years) compared to the other 5 stands ranging from 121 to 150 years of age.

Case II

When analysing the data from Case II, spectra below 900 nm were removed because of high levels of noise observed in this region. The NIR data therefore consisted of wavelength variables from 900 nm to 2500 nm.

The PLS2 – DA model was fitted with four PLS components. The regression coefficients for Norway spruce and Lutz spruce showed a strong inverse relationship. The regression coefficients for Sitka spruce were small for most of the spectral range, except from the areas around 1900 nm and 2500 nm. In these spectral areas, the regression coefficients for Norway spruce and Lutz spruce were close to zero. In the model calibration, all samples (n=47) were fitted to the correct tree species.

The overall classification performance was 94%. Two Sitka spruce specimens were predicted to the wrong groups, one was predicted into the Norway spruce group and the other was predicted into the Lutz spruce group. Hence the predictive capability for Sikta spruce is 83% while it is 100% for Lutz spruce and Norway spruce.

Discussion

The results reported from the two cases demonstrate that NIR spectroscopy combined with PLS-DA models can effectively be used to correctly classify wood with similar visual appearance. The classification models does not, however perform perfectly as we report four misclassified wood specimens in the two cases combined. This is similar to what we have found in an earlier study of Scots pine (Haartveit, *et al.* 2003). Samples from sapwood and outer heartwood are commonly close to the heartwood/sapwood transition zone as there may only be a few centimetres of sapwood. A possible explanation for the misclassifications is, therefore, that some of the reflected light had penetrated into the neighbouring wood type. The two misclassified specimens originated from a stand that was significantly older than the stands in the calibration set. This indicates a potential for generalisation as the presented model obtained correct classification for 92.5 % of the wood specimens from the stand with a large deviation in age.

In case II results showed that Sitka spruce was more difficult to classify correctly than Lutz spruce and Norway spruce. Despite the small calibration set (n=48) and the structure of the regression coefficients presented in the results, the PLS-DA models still performed well for Sitka spruce (83% correct classifications). If using a larger material for model calibration, the classification performance will most likely increase also for Sitka spruce.

Test set validation is always preferred compared to different cross validation procedures (Esbensen 2000; Kozak and Kozak 2003). In both cases we used test set validation where all observations from two (Case I) and three (Case II) stands were used as test sets. This is an approximation to true test set validation as it is only the sampling of wood samples from different stands that can be considered independent samplings. The NIR spectra

must be considered one sampling for each case. The conservative approach we have used here is as close as possible to a new and independent sampling given the available data. When data from complete stands are removed from the model calibration, the validation procedure is more reliable when compared to random or systematic selection of the test set. If allowing specimens from the same stand, or same tree, to be present in the calibration and validation sets, there is considerable risk of over-estimating the classification performance of the models.

Models with few PLS components are preferred in order to obtain a simple and robust model which is less affected by noise and sampling errors (Esbensen 2000). In Case I we used five PLS components, and in Case II we used only four PLS components. In an earlier study we used Linear Discriminant Analysis (LDA) based on Principal Components (PC) scores from a Principal Component Analysis (Flæte and Haartveit 2003). The PCs are extracted so that the total variance among the independent variables are maximised. Although the prediction performance of this model was good, it required a high number of PCs (20). It seems that the PLS approach which maximises the covariance to the dependent variables result in simpler models without reducing the prediction performance when compared to the combination of LDA and PCA.

In this study we have demonstrated two cases where NIRS combined with PLS-DA models were used to effectively classify wood with similar visual appearance. Both models showed a high prediction performance and were based on few PLS components. In Case I the NIR-spectra were obtained on the radial surfaces, while in Case II the spectra were obtained on the cross-sectional surfaces. For industrial applications there may be limitations concerning available surfaces for NIR measurements. The effect of the surface for prediction performance should therefore be further explored.

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