# Near-infrared spectroscopy: A rapid non-destructive technique for measuring wood Mechanics

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## 1. Introduction:

Wood is an important natural renewable resource; it is composed of cellulose, lignin, hemicelluloses, and minor amounts of extraneous materials (Izzekor and Fuwape 2010). Variations in the characteristics and volume of these components and differences in cellular structure make woods heavy or light, stiff or flexible, and hard or soft. It is prevalent In our everyday lives and used to manufacture, wood-frame houses, furniture railroad ties; fence posts and utility poles; fuel wood; textile fabrics, paper, and organic chemicals.

Unlike other materials it is an orthotropic and anisotropic material that is; it has unique and independent mechanical properties in the direction of three mutually perpendicular axes because of the orientation of the wood fibers and the manner in which a tree increases in diameter as it grows (Amtzen and Charles 1994, Bergman et al. 2010). It is also defined as a natural composite material with cellulose fibrils acting as reinforcing elements in an amorphous matrix of hemicelluloses and lignin. Properties vary along three mutually perpendicular axes: longitudinal, radial, and tangential. The longitudinal axis is parallel to the fiber (grain) direction, the radial axis is perpendicular to the grain direction and normal to the growth rings, and the tangential axis is perpendicular to the grain direction and tangent to the growth rings.

Although most wood properties differ in each of these three axis directions, differences between the radial and tangential axes are relatively minor when compared to differences between the radial or tangential axis and the longitudinal axis (Amtzen and Charles 1994). It is also a renewable resource with an exceptional strength-to-weight ratio and a desirable construction material showing no signs of declining utility.

## 2. Mechanical Properties of Wood Material

Mechanical properties are the characteristics of a material in response to externally applied forces. An external force is defined as any force outside of a given piece of material that tends to deform it physically (Amtzen and Charles 1994).

The mechanical strength of wood is derived from its three constituent polymers: cellulose, hemicellulose, and lignin (Kollmann and Cote 1968). All three polymers exhibit vastly different mechanical properties, and each plays a major role in wood strength. The mechanical properties of wood considered are stiffness or elasticity, tensile strength, compressive or crushing strength, shearing strength, toughness, hardness, cleavability, and resilience.

Stiffness is the ability of the material to resist deformation induced due to load, toughness is the ability of the material to absorb energy in the plastic region of the stress/strain graph, hardness is the measure of resistance to surface penetration and surface abrasion and resilience is the ability of the material to absorb energy when deformed elastically and return it when unloaded (Kretschmann 2010). The present chapter deals with the evaluation of mechanical properties i.e. modulus of elasticity (MOE), and modulus of rupture (MOR), of wood samples of *Eucalyptus tereticornis*

## 3.Non-Destructive Estimation of Wood Properties

Evaluation of the mechanical properties of wood is obtained mainly through destructive methods of experimentation as per relevant standards (Pellerin and Ross 2002). In India, most of the testing is done as per Indian slandered which are mostly derived from British and ASTM standards. Different countries have different standards (Rajput et al. 1991). However researchers around the world are working on indirect methods to evaluate timber properties (Tanasoiu et al. 2002, Schimleck 2008, Mora and Schimleck 2009).

Indirect testing or nondestructive testing (NDT) is known as the science able to assess and identify mechanical properties or defects in a piece of material or structure, without altering their end-use capabilities and then using this information to make decisions regarding appropriate applications (Pellerin and Ross 2002, Tanasoiu et al. 2002). A number of NDT techniques like ultrasonic stress wave, deflection method, electrical method, gamma radiation method or isotope method, penetration radar method, and X-ray method used in the forest products industry can be applied to control and evaluate the quality and properties of wood and wood structures (Pellerin and Ross 2002, Tanasoiu et al. 2002).

Near-infrared (NIR) technology has received considerable attention for its use in quality control and assessing wood quality and the technical review of the technology and its potential applications in wood products is summarized by So et al.(2004). The distinctive advantages of NIR over other NDT techniques are its ability to do simultaneous analysis of many parameters (Schimleck et al. 2006b, Schimleck et al. 2007, Schimleck 2008, Mora and Schimleck 2009). The other distinctive feature is its applicability to online monitoring in the industry. In fields, the portable NIR instrument and lab-based analysis make it an important tool. Easy calibration method transfer from one machine to another machine makes it a versatile tool (Meder at el. 2003, Brashaw at el. 2009).

## 4. Spectroscopic background of Near-Infra Red Spectroscopy (NIRS)

The history of near-infrared (NIR) began in the 1800 century with Herschel, who found light radiation beyond the visible spectrum (Barton 2002). But the expansion of NIR spectroscopy did not start before the 1950s from the agriculture realm into pharmaceutical, industrial processing, and imaging spectroscopy.

The NIR region spans the wavelength range 800 to 2500 nm (4000 to 12500 $cm^{-1}$) in which absorption bands correspond mainly to overtones and combinations of fundamental vibrations (Siesler 2006). Near-infrared (NIR) technology in terms of transmitted or reflected spectra of electromagnetic waves ranging from 800 to 2500 nm (4000 to 12500 $cm^{-1}$) has been mainly used for the nondestructive measurement of organic materials such as agricultural products or foods. However, it shows great potential in all facets of material assessment (for example, polymer, textile, pharmacy, petrochemical, etc.).

## 5. Use of NIR Spectroscopy to evaluate mechanical properties of wood material

Generally, the mechanical property is obtained through destructive experimentation with the help of mechanical testing machines in the laboratory. A method using an approach entirely different from conventional techniques was first introduced to non-destructive mechanical testing of wood by Hoffmeyer and Pedersen (1995) using near-infrared spectroscopy (Tsuchikawa 2007). many researchers have reported the applicability of the NIR technique to nondestructive methods of mechanical properties (Kelley et al. 2004a, Kelley et al. 2004b, Tsuchikawa et al. 2005, Fujimoto et al. 2007, 2008, Schimleck et al. 2007, Mora et al. 2008.

The potential of Near Infrared Spectroscopy (NIR) to evaluate specific mechanical characterization was the modulus of elasticity (MOE), and modulus of rupture (MOR) in bending tests has been demonstrated by a number of researchers (Mora et al. 2008, Schimleck, 2008, Schimleck et al. 2009, Hein et al. 2009, Mora and Schimleck 2010, Kothiyal and Raturi 2011).

In the continuation of mechanical properties estimation by NIR spectroscopy, Kothiyal and Raturi (2011) tried to short out the problem, regarding the limitation of NIR spectroscopy application with variation in moisture content of wood in timber yards. They obtained NIR models for predicting MOR, and MOE. The ability of NIR to measure modulus of elasticity (MOE) and modulus of rupture (MOR) is attributed to the absorbance of light by lignin and cellulose at specific wavelengths (Mclellan et al. 1991).

## 6. Chemo-metrics and multivariate model development using NIR technique

Chemo-metrics is an approach to analytical and measurement science based on the idea of indirect observation. Measurements related to the chemical composition of a substance are taken, and the value of a property of interest is inferred from them through some mathematical relation (Lavine 1998). It helps the NIR units in resolving highly overlapped and broad peaks, with high sensitivity to sample physical characteristics. NIR spectroscopy requires chemo-metrics to extract as much relevant information as possible from the analytical data (Massart et al. 1988). The analytical information contained in NIR spectra can be extracted by using various multivariate analysis techniques that relate several analytical variables (as in a NIR spectrum) to measure properties. The multivariate techniques most frequently used allow samples with similar characteristics to be grouped, in order to establish classification and determine some properties of unknown samples for qualitative and quantitative analysis respectively (Blanco and Villarroya 2002).

Without chemo-metric and multivariate methods, NIRS applications would not be possible. The chemo-metric technique covered the calibration by multiple linear regression (MLR), choosing a training set, spectral pre-treatments, tuning and validation, principal component analysis (PCA), quantitative calibration using partial least squares (PLS), principal component regression (PCR), qualitative calibration using discriminate analysis and regression methods for developing the calibration models as their use in the modeling process, those are included in all chemo-metric software packages.

A number of multivariate-analysis methods can be classified according to their purpose and their algorithms or computational procedure. The method of choice will depend on the purpose of the analysis, the characteristics of the samples, and the complexity of the system concerned (for example its non-linearity). Once models are constructed, their predictive capacity must be checked on separate sets of samples subjected to the same treatment (spectrum recording conditions and spectral pretreatments) as those used for calibration but not part of the calibration regression model. When carrying out a calibration between properties to be measured and absorbance of NIR spectra, the multivariate-regression methods most frequently used in NIR spectroscopy i.e. the principal component regression (PCR), partial least squares (PLS) and multiple linear regression (MLR) are the three best calibration methods (Agelet and Hurburgh 2010).

Principal component regression (PCR) and partial least-squares (PLS) regression both can be used in specific spectral regions or the whole spectrum, and they allow more information to be included in the calibration model. PCR uses the principal components provided by PCA to perform regression on the sample property to be predicted, while PLS finds the directions of greatest variability by considering both spectral and target-property information, with the new axes called PLS components or PLS factors (Martens and Naes 1991). In the case of multiple linear regression (MLR), it combines a set of several spectral regions or X-variables, in linear combinations, which correlate as closely as possible to a corresponding single response (property of material) or Y-vector.

In the wood material science discipline, the most popular models are PLS and PCR and both can overcome substantial multi-co linearity problems (Via et al. 2003). The PLS regression method was used for calibration model development in the present study. Before developing the calibration model, mathematical pre-treatment of spectra reduces noise or background information and increases signal quality. Generally, the most widely used pre-processing techniques can be divided into two categories: scatter-correction methods and spectral derivatives. The scatter-corrective pre-processing method includes three basic preprocessing concepts: Multiplicative Scatter Correction (MSC), Standard Normal Variate (SNV), and Normalization. The spectral derivative includes two basic preprocessing concepts: the first derivative and the second derivative. Calibration of heterogeneous material (like wood) may require broad calibration sets than homogeneous.

Some researchers have taken more than 100 wood samples for the calibration set; therefore, wide ranges of data were obtained in the calibration set (Fujimoto et al. 2008, Hein et al. 2009, 2010).

Calibration and validation statistics for each regression include the coefficient of determination ($R^2$), the root mean standard error of calibration (RMSEC), the root mean standard error of cross–validation (RMSECV), and root mean standard error of prediction (RMSEP). The final statistics to be discussed are the ratio of performance of deviation or relative predictive determinant (RPD) and Range error ratio (RER).

The coefficient of determination $R^2$ is used in the context of statistical models whose main purpose is the prediction of future outcomes on the basis of other related information. It is the proportion of variability in a data set that is accounted for by the statistical model (Steel and Torrie 1960). It provides a measure of how well future outcomes are likely to be predicted by the model.

The RMSEP value is calculated as the root mean squared difference between predictions and reference values. It is important to stress that this procedure is effective only when the noise in the reference values is negligible compared with the true prediction uncertainty. The reason for this is that prediction errors are defined with respect to the true quantities, rather than noisy reference values. The ideal situation for the perfect model is that it has no noisy reference values. Of course, this limit is not practical, but adding noise to the reference values as described by (Difoggio 1995, Coates 2002) can always approach to perfect model. Clearly, the predictions should be perfect and the only contribution to RMSEP would originate from the measurement error in the reference values. In this extreme case, RMSEP would just estimate the standard deviation (square root of the variance) of the measurement error of the reference value. It would not relate to the true prediction uncertainty.

The description of RMSECV is the same as RMSEP. The difference between statistical values of these parameters is used as a method for determining the best number of independent variables to use in building a calibration equation, based on a repetitive algorithm that selects samples from a sample set population to develop the calibration equation and then predicts on the remaining unselected samples (Difoggio 1995, Coates 2002).

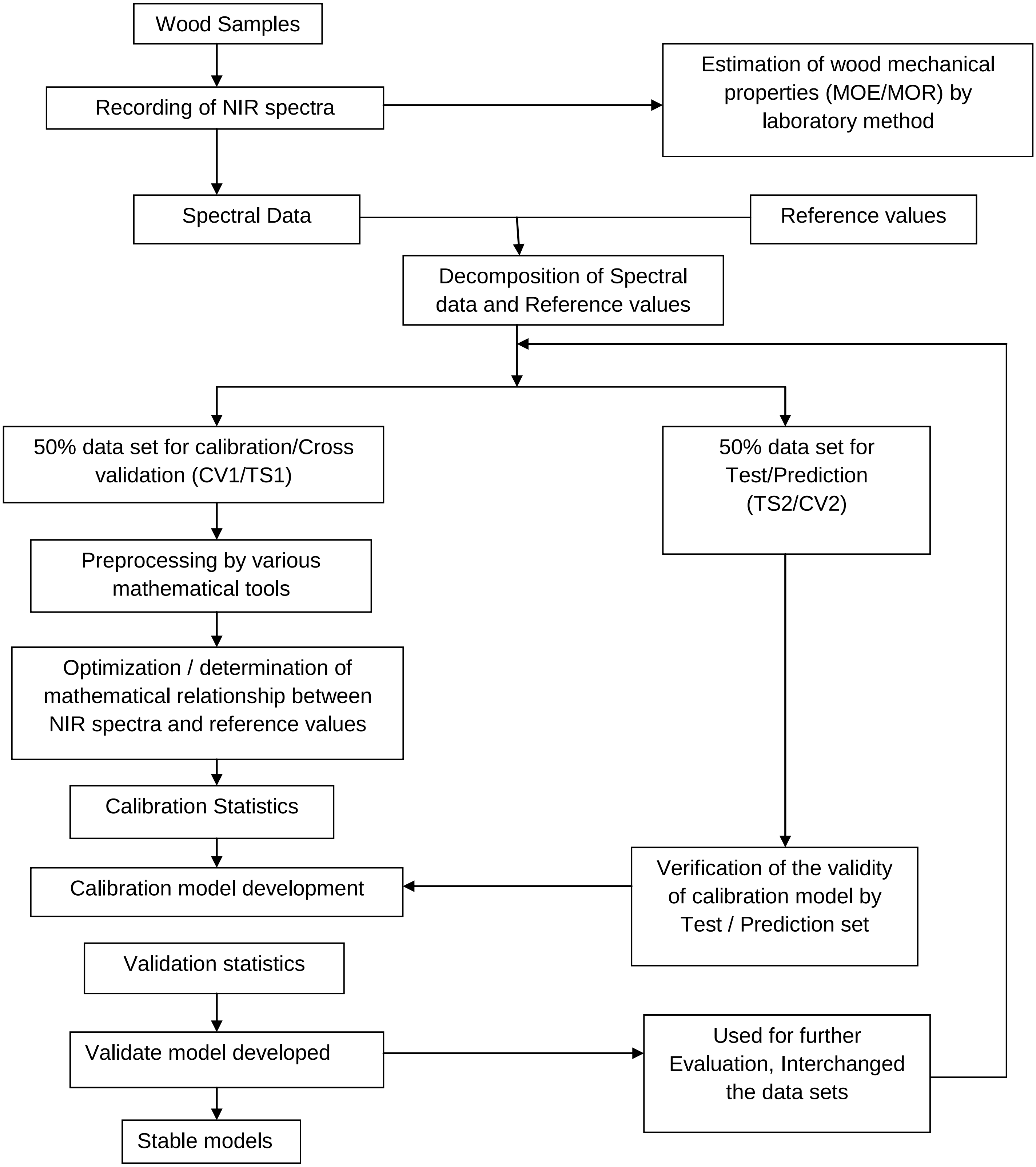
The ratio of performance to deviation (RPD: ratio of the SD of the reference results to RMSEP) is a measurement of the ability of a NIR spectroscopy model to predict a constituent. Reporting RMSEP alone may be misleading unless it is reported by comparison with the SD of the original reference data. If the RMSEP is close to the SD, then the NIRS calibration is not efficiently predicting the composition or functionality. If RMSEP = SD, the calibration is essentially predicting the population mean (Bailleres et al. 2002). The use of RER in NIR predates the appearance of RPD. Its statistics are similar to RPD, using the range of the reference values in the validation set in place of standard deviation. It is also dimensionless and also independent of the application (Fearn 2002).

These are related to the ability of the model to predict future data in relation to the initial variability of calibration data. Davies and Fearn (2006) reported the definition and application of all these terms. In the absence of a sufficient number of samples where a separate set of samples for prediction are not available other criteria are generally used (Derkyi et al. 2011) to assess the quality of a model including the root mean squares error of estimation (RMSEE), root mean square error of cross-validation (RMSECV) and the correlation coefficient of determination ($R^2$). A good model should have a low RMSEE, a low RMSECV, and a high $R^2$ between the predicted and measured values, but also a small difference between RMSEC and RMSECV. The correlation coefficient of determination ($R^2$), the most commonly used, should be higher than 0.8 for quantitative prediction. For excellent models, the RMSEE to SD ratio should be $\leq$ 0.2, where SD is the standard deviation of the reference values. If 0.2, RMSEE to SD ratio $\leq$ 0.5, quantitative predictions are possible. The SD to RMSECV ratio should be $\geq$ 2, RMSECV to RMSEE $\leq$ 1.2, and the SD to RMSCEV ratio should be $\geq$ 2.5. RMSECV can be an indication of how well an equation will predict samples that are not used to generate the calibration equation when there are insufficient external validation samples.

In the development of calibration models for the mechanical properties of wood material, many researchers used different pre-processing and statistical tools for getting excellent calibration and validation models. Thumm and Meder (2001) explored the use of spectra pretreatment, using first and second derivatives, and achieved a prediction coefficient of determinations ($R^2$) of 0.55 to 0.72 for stiffness in the bending test. Schimleck et al. (2001a) also used the first and second derivatives to help develop PLS models that provided prediction $R^2$ over 0.80 for both MOR and MOE. Modulus of elasticity (MOE), modulus of rupture (MOR) wood species have been accurately predicted by the number of researchers (Hoffmeyer and Pederson 1995, Gindl et al. 2001, Schimleck 2001a, Thumm and Meder 2001, Kelley et al. 2004a, 2004b, Tsuchikawa et al. 2005 Fujimoto et al. 2008, Viana et al. 2009, Kothiyal and Raturi 2011). They used NIR and various statistical techniques (PLS, MLR, and PCR) and also found that the calibration of green wood may be improved by using spectral pre-processing techniques.

NIR has not yet been utilized by the industry despite current research showing value as a non-destructive indicator of wood strength. The initial high cost of NIR spectrophotometers may be partially to blame. However, reduced spectral range NIR spectrophotometers, which are more economical, have also been able to accurately predict MOE and MOR. Reduced ranges from 400nm to 1100nm produced solid results (Kelley et al. 2004a). Further research involving NIR and moving samples has produced good results and the concept is promising for adaptation of spectral techniques to the production environment (Thumm and Meder 2001). The introduction of NIRS in the field of wood material science is a welcome step as more and more materials will be required for evaluation at low cost, high speed, and with improved accuracy in a non-invasive manner. Figure 1. illustrates the flow diagram of NIR models development and models evaluation for mechanical properties of wood.

**Figure 1. Flow diagram of NIR development and models Development**



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