Determination Of Wood Density And Chemical Composition With Fourier Transform Infrared Spectroscopy

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Fourier Transform Infrared (FT-IR) Spectroscopy

- Chemical bond absorb infrared radiation at a unique frequency yielding information on the molecular structure and interactions
- Diffuse reflectance infrared Fourier transform (DRIFT) technique allows solid/powdered samples to be analysed
- Rapid and non-destructive means of getting information

Experimental

- Sitka spruce: clonal (x493); Sawmill kiln-dried and fresh samples. 30 Scots pine samples (x20)
- Tropical hardwood samples (x25).
- Densities and lignin, α -cellulose and resin/extractive contents were measured using standard methods.
- Diffuse reflectance technique was used to collect IR spectra from the ground wood samples.
- Multivariate data analysis (PLS) was used to establish relationships between IR spectral data and wood density and chemical composition.

Wood density

Lignin, α -cellulose and resin content

- Models of lignin, α -cellulose and extractive/resin contents were constructed.
- The lignin model gave a fit, RMSEE and RMSEP of 0.78, 1.0 and 1.6, respectively. The corresponding α -cellulose values were 0.65, 1.6 and 2.9, respectively.

Lignin content, % (w/w)



The model gave a fit of 0.86 and residual mean squares error of estimation (RMSEE) of 35 and was externally validated using 250 samples. RMSEP (prediction) for the test set data was 56. The model operates well as a tool to rapidly distinguish between high and low density samples.

Density (measured), (kg/m3)



Fig.1 Calibration between wood density and FT-IR spectral data.

Spectral differences between low and high density samples originate from differences in polysaccharide and lignin composition. This is reflected below with positive and negative bands relating to high and low density samples respectively (Fig. 2). Positive IR absorptions are mainly due to the vibrations of polysaccharides, whereas negative signals are associated with lignin.

Lignin content (predicted), % (w/w)

Fig.3 Calibration between measured and predicted lignin content on the basis of DRIFT spectra.

PLS calibration between wood resin content and DRIFT data constructed from Sitka spruce data set (Fig. 4) had a good fit and predictive power (R² 0.94 and RMSEP of 0.93).

Wood resin content (measured), % (w/w)



Conclusions

 FT-IR spectroscopy proved to be a successful tool to estimate wood density and chemical composition. • The statistical models revealed specific wavelengths that were intimately related to wood density. • The use of only selected wavelengths in detectors should allow portable mid-infrared devices to be simpler, robust and economical.



Fig. 2. PLS regression coefficients of the density model showing spectral differences due to density variation.

- Accurate and portable spectrometers would allow tree breeders and foresters to screen wood for density and chemical composition in situ.
- FT-IR spectrometers could also be used for analysis in sawmills to determine raw materials and/or the sawn timber.

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