Identification and characterization of Estonian wood using ATR-FTIR spectroscopy combined with multivariate analysis

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The push towards greener alternatives brings lignin into consideration as a sustainable starting material. If lignin is considered as a waste-product, the quality of extracted lignin will be too low to valorize it fully. There are pretreatments that extract lignin before other industrial processes, but the extracted lignin might not be easy to degrade and functionalize because it is extracted in conditions which causes the lignin to repolymerize and condense. That is why newer and improved pretreatments are needed.[1] To compare the lignins that are collected in different conditions, better, faster, cheaper, and more reliable analytical methods are needed. Analytical chemistry provides vital information about the process, its yield and product purity. Currently, most methods are to do with lignin functional groups, such as hydroxyl, methoxy, carbonyl and carboxyl groups. Elemental analysis, infrared spectroscopy and nuclear magnetic resonance spectroscopy are used to characterize lignin. Spectroscopic methods such as infrared spectroscopy are often used to build chemometric models because of the ease of use and nondestructive nature.[2]

Developing new analytical methods is crucial for characterization of lignocellulosic biomass and quality control for valorized products. Composition of lignocellulosic biomass was determined using classical "wet chemistry" and spectroscopic methods and multivariate data was analyzed using chemometric methods. Klason lignin[3,4] and extractives content[5] were measured gravimetrically in 90 wood samples. The accuracy of Klason method was determined using a certified reference material.

It was determined that birch contains 25,8 ± 3,2 % of lignin and 3,5 ± 0,8 % of extractives, spruce contained 31,1 ± 3,0 % of lignin and 2,0 ± 0,7 % of extractives and pine contained 32,2 ± 3,0 % of lignin and 6,1 ± 3,0 % of extractives. There results were in compliance with data gathered from the literature. Infrared spectra were measured for all samples and the data was used to conduct a PCA analysis, which showed that the samples clearly separated to hardwood and softwood clusters, but the area of logging and wood composition had no correlation. Acid soluble lignin, Klason lignin and extractives amounts were used to build a PLSR model. Five PLS components were used, and the prediction performance was determined using standard cross-validation. PLS model was able to predict ASL, KL and EA content with a correlation coefficient of R^2~0,9 creating the model and R^2 0,6-0,8 cross-validating. The PLSR model was able to predict ASL, KL and EA concentrations with a relatively low standard deviation (up to 15%) and the concentrations were close to measured concentrations. This shows that multivariate data analysis can be used to replace classical chemistry methods, such as Klason method, in day-to-day wood analysis.

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