APPLICATION OF FT-NIR IN POPLAR CHEMICAL ANALYSIS

Jianxing Zhang,¹ Evandro Novaes, Gary F. Peter, and Matias Kirst

¹School of Forest Resources and Conservation, University of Florida, Gainesville, FL

Genetic analysis of wood chemical composition is limited by the cost and throughput of direct analytical methods. Indirect methods such as <u>Fourier transform</u> near infrared (FT-NIR) offer an alternative for rapid, low cost method. In FT-NIR, calibration models and their predictions are typically developed and validated from small sample sets. These models are subsequently used to estimate wood chemical composition from larger sets of new samples (e.g., Sykes et al., 2006. Ann. For. Sci. 63, 897-904). However, no direct comparison of direct and indirect estimates of wood chemical composition and the genetic parameter estimates have been reported for the same population. Here we compare for a single poplar family genetic parameter estimates obtained for wood chemical composition with data from pyrolysis molecular beam mass spectrometry (pyMBMS) and FT-NIR.

Over two thousand young greenhouse grown wood samples were analyzed for chemical composition with pyMBMS (Novaes et al. 2009. New Phytologist, 182, 878-890). We randomly selected 496 samples to build a Fourier transform near infrared (FT-NIR) calibration and validate a model based on partial least square for lignin percent, corrected lignin, G-lignin, S-lignin, S/G ratio and sugars (C5 and C6). A FT-NIR spectrometer, equipped with an X-Y stage auto-sampler was used to improve the scanning efficiency. The sample set was randomly divided into calibration (397) and prediction (99) sets. The coefficient of determination (\mathbb{R}^2) for the calibrations ranged from 0.54 to 0.91, and the prediction model \mathbb{R}^2 ranged from 0.46-0.88. Stronger calibration and prediction statistics were obtained with lignin compared with carbohydrates. For lignin the best prediction ($\mathbb{R}^2 = 0.88$) was obtained for lignin percent. For carbohydrates, the strongest prediction statistics ($\mathbb{R}^2 = 0.71$) were obtained for the m/z 144 ion which comes from cellulose. Genetic analysis of pyMBMS data and FT-NIR predictions will be compared to evaluate the utility of the indirect FT-NIR method relative to the direct pyMBMS method for parameter estimates.