Role of chemometrics for at-field application of NIR spectroscopy to predict sugarcane enzymatic hydrolysis performance

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During the last years, the supply of sustainable energy from lignocellulosic feedstock has become a major concern. In this context, methodologies for rapid characterization of this complex material, which may be applied in the industrial environment, are relevant for routine bioprocess operation. If the characterization procedure can be associated with knowledge-based models inferring yields of biochemical conversion (enzymatic hydrolysis), a significant impact on process economics may result. A rapid analytical method, properly calibrated by chemiometrics, is fundamental for further creation of a consistent library of data. These tools may even be used as selection criteria between competitive technological options for processing cellulosic material into ethanol. Thus, this work presents a quick method for analyzing the chemical composition of sugarcane bagasse, by using near-infrared (NIR) spectroscopy coupled with multivariate analysis. NIR sugarcane spectra were collected from 42 samples, which were obtained from three different pretreatment methods (organosolv, sodium hydroxide and aqueous ammonia). A rapid calibration model is put forth to predict cellulose, hemicellulose and lignin yields of a variety of pretreated sugarcane samples. NIR spectra are correlated to compositional data produced using traditional wet chemical analysis. An exploratory principal component analysis (PCA) of a NIR spectral data matrix of the pretreated sugarcane samples showed a clear trend along PC1, similar to that found from the chemical composition. On the other hand, a broad-based model hypothesis that a single NIR predictive model can be developed to analyze multiple types of pretreated sugarcane feedstock is reported. Both cross-validation and independent validation results showed that the developed broad-based model is promising for future chemical prediction of other pretreated samples. Finally, this paper illustrates the crucial role of chemometrics in replacing laborious analyses for inferring sugarcane hydrolysis performance (based on wet chemical measurements), by a rapid near infrared (NIR) spectroscopic methodology in industrial screening applications.