Abstract

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Determination of glucose and ethanol in bioethanol production by near infrared spectroscopy and chemometrics

The concentrations of glucose and ethanol in substrates from bioethanol processes have been modeled by near infrared (NIR) spectroscopy data. NIR spectra were acquired in the wavelength range of 1100–2300 nm by means of a transflectance probe for measurements in liquid samples.

For building of regression models a genetic algorithm has been applied for variable selection, and partial least-squares (PLS) regression for creation of linear models.

A realistic estimation of the prediction performance of the models was obtained by a repeated double cross-validation (rdCV). Reduced data sets with only 15 variables showed improved prediction qualities, in comparison with models containing 235 variables, particularly for the determination of the ethanol concentration in distillation residues (stillages).

The squared correlation coefficient, R^2, between the concentrations obtained by HPLC analysis and the concentrations derived from NIR data (using 15 selected wavelengths, test set samples) was 0.999 for ethanol in stillage, and 0.977 for glucose in mash. The standard deviation of prediction errors, SEP, obtained from test set samples was 0.6 g L^{-1} for ethanol (2% of the mean ethanol concentration), and 2.0 g L^{-1} for glucose (9.6% of the mean glucose concentration).