Applicability of near-infrared spectroscopy for process monitoring in bioethanol production

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Abstract. Near-infrared spectroscopy and chemometrics were applied for the characterization, classification, and quantification of decisive parameters in bioethanol production processes (Fig.1). In bioethanol production chemically undefined multiple substrates with highly varying complexity due to different feedstock or enzymatic reactions pose a challenge to process analytics. By screening experiments the feasibility of measuring particular properties by NIR spectroscopy was investigated.

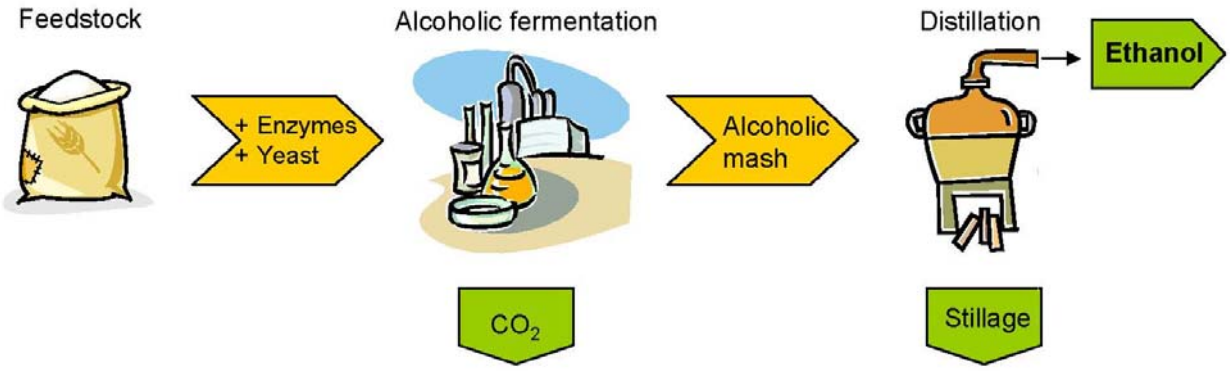

Fig. 1. Schematics of the bioethanol process

Despite the similarity of NIR absorbance spectra (Fig. 2 here shown for 216 different mash and stillage samples), several compounds could be quantified by appropriate multivariate data analysis. The mainly application-oriented project also required the development of chemometric methods and software (in the programming environment “R”) [2,3].

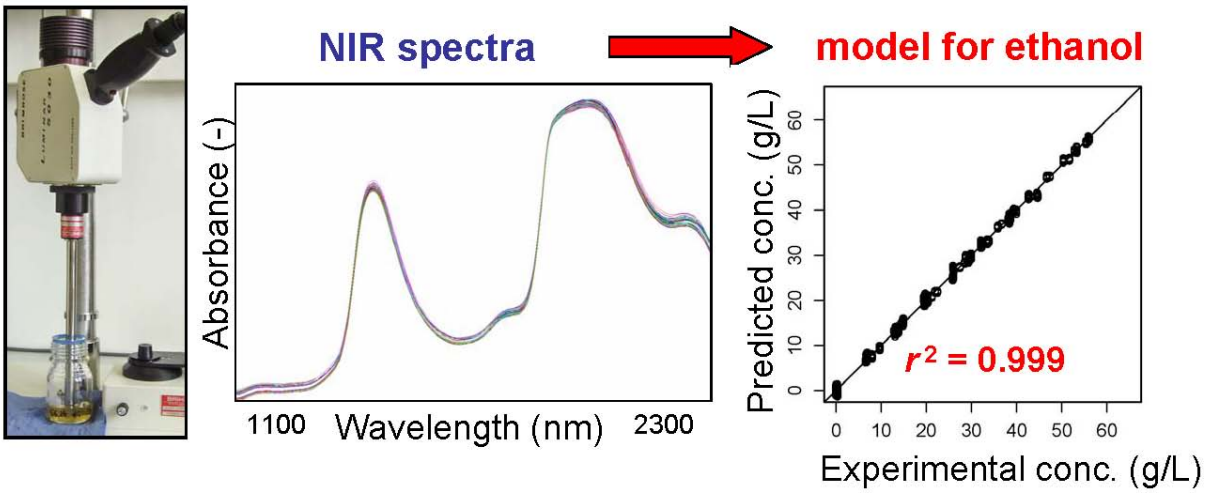

Fig. 2. From samples to NIR data and to models predicting concentrations.

Near-infrared (NIR) spectroscopy and chemometrics were successfully applied to characterize bioethanol feedstock (corn, wheat, rye, triticale, and barley), and process broths. Calibration models were built and validated for moisture, protein, and starch in the feedstock material, and for glucose, ethanol, glycerol, lactic acid, acetic acid, maltose, fructose, and arabinose in the processed broths. These broths were prepared in laboratory experiments: The grinded cereal samples were fermented to alcoholic broths ('mash'), which were divided into an ethanol fraction and the residual fraction 'stillage' by distillation. The NIR technology together with chemometrics proved itself beneficial for fast monitoring of the current state of the bioethanol process, primarily for higher concentrated substances (> 1 g/l).

[1] B. Liebmann, A. Friedl, K. Varmuza: Determination of glucose and ethanol in bioethanol production by near infrared spectroscopy and chemometrics. *Analytica Chimica Acta*, 642 (2009), 171-178

[2] P. Filzmoser, B. Liebmann, K. Varmuza: Repeated Double Cross Validation. *Journal of Chemometrics*, 23 (2009) 160-171

[3] B. Liebmann, P. Filzmoser, K. Varmuza: Robust and Classical PLS Regression compared. *Journal of Chemometrics*, 24 (2010) 111-120