

T13. PLS2 regression as a tool for selection of optimal analytical modality — a closer look at beer brewing process analysis with alternative spectroscopic data types

Michael Madsen and Kim H. Esbensen

ACABS research group, Aalborg University, campus Esbjerg, Denmark

Intelligent use of modern process analysers allows process technicians and engineers to look deep into the dynamic behaviour of production systems. This opens up for a plurality of new possibilities with respect to process optimisation. Oftentimes, several instruments representing different technologies and price classes are able to decipher relevant process information simultaneously. The question then is: *how to* choose between available technologies without compromising the quality and usability of the data. We apply PLS2 modelling to quantify the relative merits of competing, or complementing, analytical modalities.

We here present results from a feasibility study, where Fourier Transform Near InfraRed (FT-NIR), Fourier Transform Mid InfraRed (FT-MIR), and Raman laser spectroscopy were applied on the same set of samples obtained from a pilot-scale beer brewing process. Quantitative PLS1 models were constructed for the most interesting parameters, namely ethanol, maltose, and total sugar. Models were naturally validated with appropriate test sets. The same three set of multivariate spectra were subsequently related to one another using a sequential PLS2 approach allowing to quantify the proportion of *unique* vs. *joint* information in each spectral data type. These results reveal new quantitative interrelationships between NIR, MIR and Raman spectral information on biological systems.