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Why can the glucose concentration during cultivations be predicted from fluorescence spectra?

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1. Introduction

Fluorescence spectroscopy is a powerful and convenient method for monitoring and controlling biotechnical processes. If cells are involved, certain fluorophors permit an insight in the cell's metabolism. Figure 1 provides an impression about the great amount of information contained in fluorescence spectra.

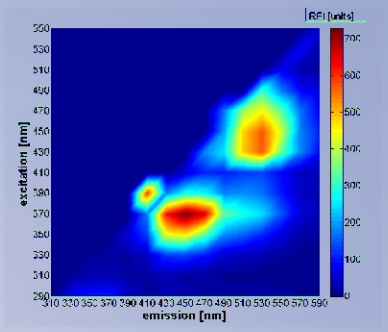

Figure 1: Difference spectrum of a Cultivation of *S.cerevisiae*

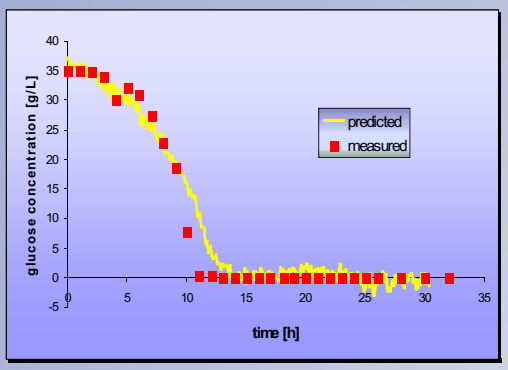

Figure 2: Prediction of the glucose concentration, RMSEP = 7,3 %

2. Chemometric models

Evaluation of fluorescence spectra is most suitable performed by using chemometric methods, for example PCA and PLS. The models obtained by these methods can then be used with other spectra data for the prediction of e. g. the concentrations of glucose and biomass. The glucose concentration of a cultivation of *Saccharomyces cerevisae* is shown in figure 2, predicted out of spectra data with models created with another data set. The Biomass contains several fluorescent constituents, whereas glucose is no fluorophor. In spite of that, why is modeling based on fluorescence spectra possible?

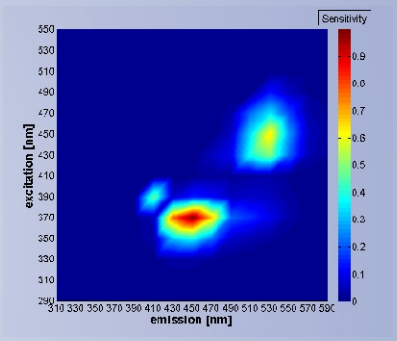

Figure 3: Sensitivity spectrum for the prediction of the biomass concentration

.3. Sensitivity analysis

Each 2D-fluorescence spectrum consists of 120 different wavelength combinations. To analyze the influence of the biomass on the modeling of the glucose concentration a sensitivity analysis can be performed. The sensitivity spectrum is shown in figure 3. The criteria for the sensitivity is the root mean square error of prediction (RMSEP) after gradual modifying fluorescence intensities of each wavelength combination.

Figure 4 and 5 show the errors of prediction of the biomass and the glucose concentration after removing an increasing number of significant wavelength combinations. Both figures show similar characteristics which indicates that both process parameters are predicted out of similar wavelength combinations.

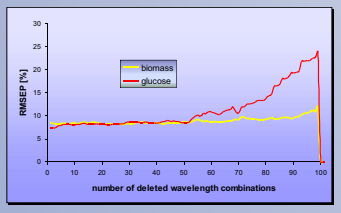

Figure 4: Variation of the RMSEP with increasing number of removed wavelength combinations for biomass prediction

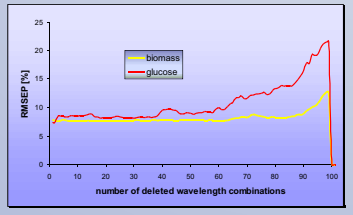

Figure 5: Variation of the RMSEP with increasing number of removed wavelength combinations for glucose prediction

4. Prediction with modified spectra

With the new created reduced spectra, new models can be calculated. The predictions of the biomass and glucose concentrations are demonstrated in figure 6 and 7.

5. Conclusion

- Glucose and biomass concentration can be predicted of fluorescence spectra
- Significant wavelength combinations for the prediction of biomass and glucose were identified separately

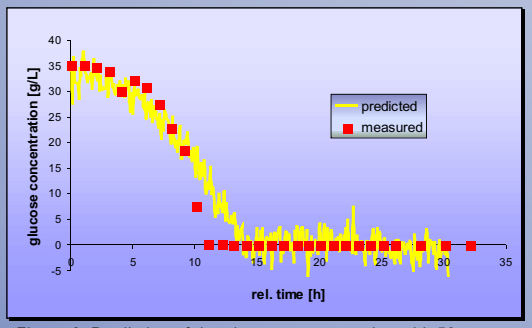

Figure 6: Prediction of the glucose concentration with 50 wavelength combinations, RMSEP = 10,6 %

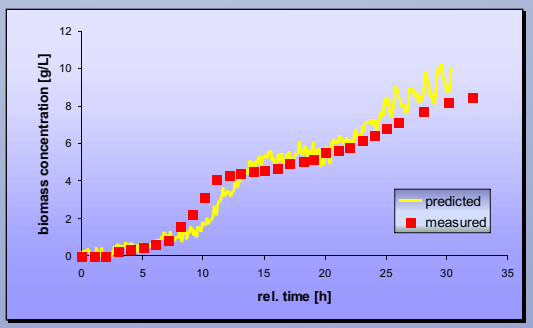

Figure 7: Prediction of the biomass concentration with 50 wavelength combinations, RMSEP = 9,2 %

- Decisive information for the prediction can not be separated. This indicates that glucose is predicted of fluorescence spectra indirectly over the biomass concentration