DEPARTMENT OF FOOD SCIENCE
FACULTY OF SCIENCE
UNIVERSITY OF COPENHAGEN

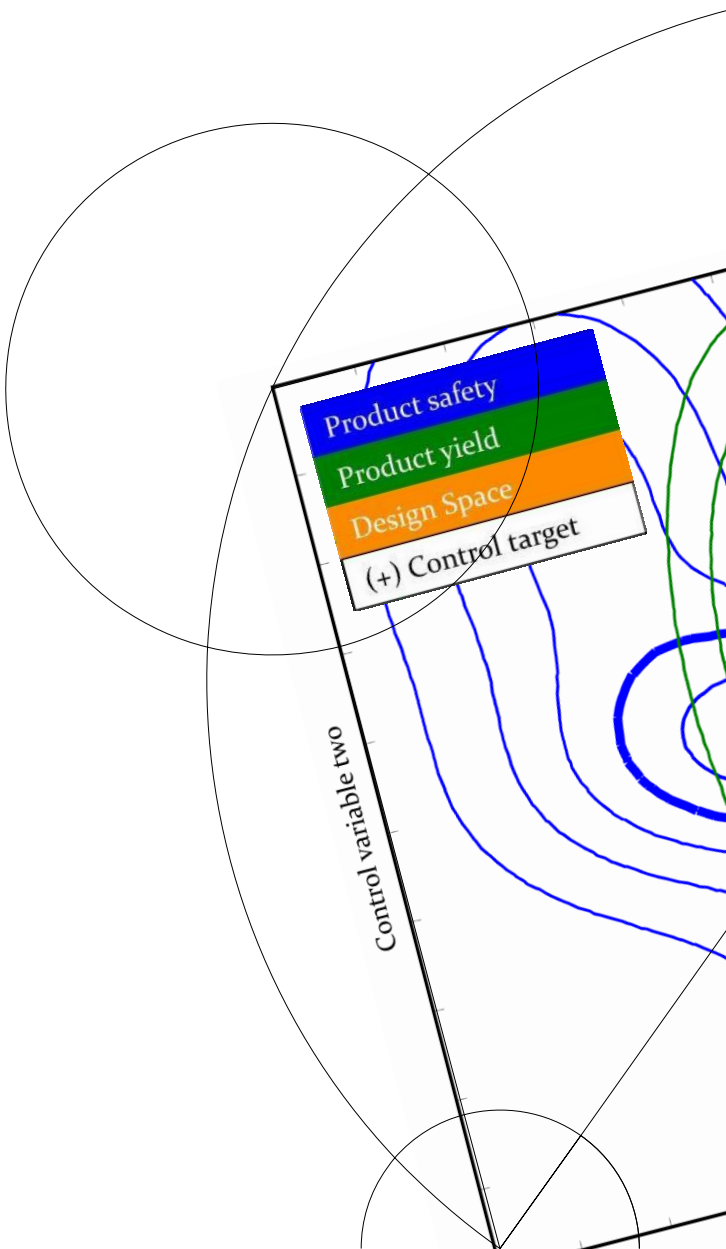
Invitation to PhD defense

Tuesday July 10th 2012 at 10:00
Auditorium A1-01.01 (Festauditoriet), Bülowsvej 17, Frederiksberg C

Title

Dynamic Models and Chemometric Tools for Process Monitoring

PhD Thesis by
Jonas Hoeg Thygesen · 2012



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ABSTRACT

The food- and pharma-industry is under an ever increasing demand for reduction in energy use, optimal production planning and efficient utilization of raw materials. This has led to the concepts of Quality by Design (QbD) and Process Analytical Technology (PAT). The aim of QbD is to use PAT-tools for obtaining greater process knowledge such that the manufacturer may move away from end-point testing of products, towards building quality into process and thus the products (hence the name Quality by Design). The purpose of this PhD project was to show how spectroscopy based PAT-tools in combination with dynamic predictive models may bring these goals closer to reality. The work presented in this thesis covers the three years research which was also published in four papers:

Paper I investigated how three-way calibrations for Excitation-Emission Matrix (EEM)-fluorescence spectroscopy could be transferred. The study showed that it was possible to develop simple, intuitive transfer methods for three-way EEM fluorescence calibrations. The paper thereby illustrated how three-way EEM fluorescence calibration made in an off-line setting (i.e. in the laboratory) with ease could be transferred to an on-line application.

Paper II introduced the state space model and showed how so-called subspace methods allowed state space modelling without *a-priori* assumptions on model shape/form, thereby enabling modelling of the process without the requirement of any prior knowledge on the underlying physics or chemistry.

Paper III elaborated further on the conclusions from **Paper II.** In this paper a combination of state space models, subspace methods and Kalman filters were shown to have the potential as a versatile tool in batch process modelling and monitoring.

Paper IV presented further studies on the model system introduced in **Paper III.** The paper illustrated what is also known as so-called grey box modelling: Modelling in the case where the physics and chemistry governing the process is known or assumed to be known to some extent. In **Paper IV** it was shown how the *a-priori* knowledge on the reaction kinetics governing the process could be implemented during PARAFAC modeling.

The different statistical/chemometric models included in this thesis made it possible to answer different types of questions. The only method able to answer all three questions: *"Where is the process now?"*, *"Where did the process come from?"* and "*Where is the process going?"* was the state space/Kalman method presented in **Paper II** and **III.** The possibility of predicting future process characteristics and variable trajectories opens for the option of model predictive control which in turn may bring the goal of QbD closer to reality.