23rd IFIP Conference on Modelling and Optimization

Invited Session

# Optimization of Dynamic Systems in Chemical Engineering II

Organizer: L. T. Biegler, University of Heidelberg (D) and Carnegie Mellon University (USA), lb01@andrew.cmu.edu

1. *Robust Optimum Experimental Design Methods with Application to Parameter Estimation in Chemistry and Chemical Engineering* - Ekaterina Kostina, University of Marburg (D), Ekaterina.Kostina@iwr.uni-heidelberg.de

2. *Optimizing Control of a Reactive SMB Process* - Achim Küpper and Sebastian Engell University of Dortmund (D), sebastian.engell@bci.uni-dortmund.de

3. *Interior-Point Quasi-Sequential Approach and Application to the Optimization of the Tennessee Eastman Process* - H. Gerbracht, P. Li, W. R. Hong TU Ilmenau (D), Pu.Li@tu-ilmenau.de

4. *Tools and languages for modeling and optimization of large scale dynamical systems* - Johan Åkesson, Lund University (S), jakesson@control.lth.se

Abstracts of all of these talks are given below.

## Robust Optimum Experimental Design Methods with Application to Parameter Estimation in Chemistry and Chemical Engineering

Prof. Ekaterina Kostina
University of Marburg

Estimating model parameters from experimental data is crucial to reliably simulate dynamic processes. In practical applications, however, it often appears that the experiments performed to obtain necessary measurements are expensive, but nevertheless do not guarantee sufficient identifiability. The optimization of one or more dynamic experiments in order to maximize the accuracy of the results of a parameter estimation subject to cost and other technical inequality constraints leads to very complex non-standard optimal control problems. One of the difficulties is that the objective function is a function of a covariance matrix and therefore already depends on a generalized inverse of the Jacobian of the underlying parameter estimation problem. Another difficulty is that the optimization results depend strongly on the assumed values of parameters which are only known to lie in a - possibly large - confidence region. Hence, robust optimal experiments are required that solve worst-case (min-max) optimization problems. We suggest new efficient solution methods for such problems. Numerical results for real-life applications from chemistry and chemical engineering will be presented.

## Optimizing Control of a Reactive SMB Process

Achim Küpper and Sebastian Engell
Universität Dortmund

In this contribution, a non-linear optimization-based control strategy for the so-called Hashimoto SMB process that combines reaction and continuous chromatographic separation is presented and results of the application to a pilot plant are shown.
The controller computes optimal control variables (flow rates and the switching time) such that an economic objective is optimized over a moving horizon. The purity requirements of the product streams are implemented as constraints and not as controlled variables. High product purities are handled by appropriate scaling of the variables to enable piecewise constant error feedback. Simulative and experimental results are presented for the example of the racemization of Tröger's base.

# Interior-Point Quasi-Sequential Approach and Application to the Optimization of the Tennessee-Eastman-Process

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In this contribution, we consider the extension of the quasi-sequential approach by integrating the interior-point method. The quasi-sequential approach is suitable for solving large-scale dynamic optimization problems with path constraints on state variables. It utilizes advantages of both simultaneous approaches (where a complete discretization for both states and controls is adopted) and sequential approaches (where a model integration step is used for eliminating the states and equalities). Furthermore, the elimination of equality constraints simplifies the line-search problem considerably and therefore larger steps can be taken towards the optimum.

An active-set strategy has been used in our quasi-sequential approach until now. It is well-known that this strategy will be inefficient for problems with a large number of inequality constraints. Therefore, in the current work this active-set strategy is replaced by the interior-point method. This modification leads to a considerable reduction of computational costs in situations where the number of active constraints is high. A comparison of the efficiency will be made by applying both alternatives of the quasi-sequential approach to the Tennessee-Eastman-Process.

# Tools and languages for modeling and optimization of large scale dynamical systems

Johan Åkesson

High level modeling languages are receiving increased industrial and academic interest within several domains, such as chemical engineering, thermo-fluid systems, power systems and automotive systems. One such language is Modelica (www.modelica.org). Modelica is an open language which is specifically targeted at multi-domain modeling and model re-use. Key features of Modelica are object oriented modeling, declarative equation modeling, a software component model enabling a-causal connections of sub models and support for hybrid/discrete behaviour. These features have proven very applicable to a wide range of large scale applications in various fields.

While there exist very efficient software tools for simulation of Modelica models, e.g. Dymola (www.dynasim.com), tool support for static and dynamic optimization is generally weak. Also, specification of optimization problems is not supported by Modelica. Since Modelica models represent an increasingly important asset for many companies, it is of interest to investigate how Modelica models can be used also for optimization, utilizing cutting edge numerical algorithms, in order to increase return of investment.

This contribution gives an overview of a project targeted at i) define an extension of Modelica, Optimica, which enables high level formulation of optimization problems, ii) development of prototype tools for translating a Modelica model and a complimentary Optimica description into a representation suited for numerical algorithms and iii) performing case studies demonstrating the potential of the concept. This project integrates dynamical modeling and optimization with computer science and numerical algorithms. One of the main benefits of the suggested approach is that the high level descriptions are automatically translated into an intermediate representation by the compiler front-end. This intermediate representation can then be translated further to interface with different numerical algorithms. The user is therefore relieved of the burden of managing the, often cumbersome, API:s of numerical algorithms. The flexibility of the architecture also enables the user to select a particular algorithm which is most suitable for the problem at hand.

A first version of the Optimica extension has recently been defined. In addition, a prototype compiler supporting a subset of Modelica has been developed. The compiler enables translation of the high level Modelica and Optimica descriptions into the language AMPL, where the continuous dynamical states have been transcribed by means of a simultaneous optimization approach based on collocation over finite elements. The resulting optimization problem can then be solved by an NLP code for large scale problems, such as IPOPT. The tools have been used to find optimal start-up trajectories for a plate reactor, (see ``Dynamic optimization of a plate reactor start-up supported by Modelica-based code generation software", Staffan Haugwitz and Johan Åkesson, submitted to DYCOPS 2007).