

KoMSO Challenge Workshop

“Challenges for Mathematical Modeling, Simulation and Optimization for Advanced Process Control of Batch Processes“

February 9-10, 2017

IWR – Heidelberg University

Mathematikon, INF 205, 69120 Heidelberg

1 Jumping-off Point

Batch processes are an important way of manufacturing chemicals. They are particularly important for the production of specialty chemicals due to their flexibility, simplicity and low investment costs.

The workshop discussed opportunities and challenges to improve the operation of batch processes in the framework of Real Time Optimization (RTO) and of Nonlinear Model Predictive Control (NMPC). This included newly developed models of reaction kinetics, new sensors and new fast mathematical optimization methods for process operation. The effects of model-based optimizing control were demonstrated by introducing problems from several application areas, e.g. polymerization processes.

The workshop served as platform to bring together representatives from both academia and industry in order to determine mathematical challenges of common interest, to improve and integrate process control solutions for applications across various industries, and to foster synergies and collaborations. Presentations and posters included research from different projects, among others the EU projects RECOBA and MOBOCON, as well as the BMBF project GOSSIP.

2 Challenge Workshop

The event was jointly organized by KoMSO and the Interdisciplinary Center for Scientific Computing (IWR) at Heidelberg University, as well as funded by BASF SE, the Heidelberg Collaboratory for Industrial Optimization (HCO) at Heidelberg University, and the Accompanying Network Activities Project IMNET (Federal Ministry of Education and Research, BMBF).

The speakers and participants included industry representatives from ABB AG, Anwendungs Software Systeme Schröder GmbH, BASF SE, Cybernetica AS, Evonik Technology & Infrastructure GmbH, GoSilico GmbH, ORDINAL Software, and TLK Energy GmbH. In addition, representatives from the following institutions participated and/or presented in the workshop: Automatic Control Lab EPFL, Fraunhofer ITWM Kaiserslautern, Heidelberg University, Karlsruhe Institute of Technology KIT, Laboratoire d'Automatique EPFL, MPI Magdeburg, POLYMAT - University of the Basque Country, RWTH Aachen, TU Berlin, Trier University, TU Dortmund, TU Kaiserslautern, Tulane University, University of Limerick, University of Chemistry and Technology Prague, and VDEh-Betriebsforschungsinstitut BFI.

3 Major Topics

The discussion concentrated on the question of how to design and operate batch processes in an optimal way, and develop and use tools of Mathematical Modeling, Simulation and Optimization (MSO) for applications in industrial practice:

- RTO applications in chemical engineering, polymerization, steelmaking, food production, etc.
- quantitative modeling for use in RTO
- development of sensors for optimizing control tasks
- advanced numerical methods for RTO and NMPC
- approaches for quantification and compensation of uncertainties in process operation

It became apparent during the workshop that MSO methods have shown high potential for improving batch process design and operation, but that there is still a gap between tools and methods available in academia and those both applied and needed in industry.

4 Challenges

Numerous topics for research projects have been identified during presentations and discussions. The participants of the workshop clearly stated that there is a need to investigate physical modeling of industrial processes and to further develop MSO tools for optimizing control.

To be more precise, *Mathematical MSO for Advanced Process Control of Batch Processes* requires the development of novel methods that

- support the establishing of models suitable for RTO of complex processes
- estimate system parameters and states in nonlinear dynamic models in real time
- can perform quantification of uncertainties and disturbances
- can treat dual control problems efficiently
- take into account constraints to ensure feasibility and safety of operation
- allow for robust operation of processes under uncertainties
- etc.

A big challenge is the development of MSO tools that cover quantitative modeling for RTO, embedded algorithms for fast and reliable parameter and state estimation, and RTO under uncertainties – and are easy to use in practice and allow for optimizing not only single production units but also even a plant-wide operation.

5 Outlook

All participants agreed that the workshop offered a much-needed platform to raise awareness of benefits that are possible by exploiting the potential of RTO and NMPC. The participants realized that the two-day workshop was too short to discuss all relevant topics in sufficient detail. It has been suggested to organize a follow-up conference and to investigate possibilities for setting up specific joint research projects.