



EC's Framework Programme for Research and Innovation Horizon 2020 (2014-2020)
Grant agreement no. 636820

Cross-sectorial real-time sensing, advanced control and optimisation of batch processes saving energy and raw materials (RECOBA)

Start of the project: Jan 1st, 2015
Duration: 36 month

Midterm dissemination event: exploitation workshop 2

Due date: August 31, 2016
Actual submission date: Feb. 20, 2017

Lead contractor for this deliverable: BASF

Author:

Company	Name
BASF	Omar Naeem, Bettina Böttcher
TKSE	
ELKEM	
UCAM	
RWTH	
VSCHT	
PMAT	
BFI	
CYB	
MINKON	

Dissimination level

- PU public
- PP restricted to other programme participants (incl. the Commission Services)
- RE restricted to a group specified by the consortium (incl. the Commission Services)
- CO Confidential, only for members of the consortium (incl. the Commission Services)



CONTENT

1	Objectives.....	2
2	Agenda.....	3
3	Result.....	4

1 Objectives

All companies of the European process industry are facing the same challenges: on the one hand product quality has to be improved and at the same time production costs have to be decreased to be competitive on the world market. On the other hand the resource and energy efficiency of products and processes has to be improved to lower their ecological footprint. This is independent of the industrial sector, it is true for the cement industry as well as for the food or copper industry. That means, these are cross-sectorial challenges. To create awareness of the project's effort in other industry sectors than the involved, partners are planning a challenge workshop in cooperation with KoMSO (Committee for Mathematical Modeling, Simulation and Optimization) as midterm dissemination event.

KoMSO serves as network within the "Mathematics for Innovations in Industry and Services" program established by the Federal Ministry of Education and Research (BMBF). KoMSO unites the triad of mathematical modeling, simulation and optimization as new field of technology in research and development to reinforce the innovational strength of Germany as a location of technology, but is also part of the European Service Network of Mathematics for Industry and Innovation (EU-MATHS-IN), an initiative to facilitate mathematics for industry in Europe. This characterises KoMSO as appropriate partner for the workshop.

The aim of this workshop was 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.

2 Agenda



KoMSO Challenge Workshop

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

Tentative Schedule

Thursday – February 9, 2017

12:00 Arrival, Registration, Lunch

13:00 **Address of Welcome**
Hans Georg Bock (IWR, Heidelberg University)

13:15 **Optimal Operation of Batch Processes under Model Uncertainty**
Sebastian Engell (TU Dortmund)

13:45 **Fully Automatic Control of Batch and Semi-batch Polymerization Reactions using Automatic Continuous Online Monitoring of Polymerization Reactions with a Control Interface (ACOMP/CI)**
Wayne F. Reed (Tulane University)

14:15 **Fast Hybrid Monte Carlo Model for Semi-batch Emulsion Copolymerization**
Thomas Chaloupka (University of Chemistry and Technology Prague)

14:45 Group Photo / Coffee Break

15:15 **Software for Batch Optimization with Focus on Reduction of Energy Consumption and Material Losses**
Philippe Allot (ORDINAL Software)

15:45 **Recent Advances in Nonlinear Model Predictive Control**
Hans Georg Bock (IWR, Heidelberg University)

16:15 **Mathematical Modeling and Model-based Real-time Control Tools for Liquid Steelmaking Processes**
Bernd Kleimt (VDEh-Betriebsforschungsinstitut)

16:45 Poster Session & Coffee Break

Fast Hybrid Monte Carlo Model for Semi-batch Emulsion Copolymerization
Thomas Chaloupka (University of Chemistry and Technology Prague)

Challenges in Online Monitoring and Model Predictive Control of a Semi-batch Polymerization Process
Johannes Faust and Preet J. Joy (RWTH Aachen)

Accelerating NMPC by Simultaneous NMPC and MHE
Ekaterina A. Kostina (IWR, Heidelberg University)

Moving Horizon Estimation - a Powerful Tool for Online State and Parameter Estimation in Nonlinear Dynamic Systems
Tom Kraus (IWR, Heidelberg University)



3 Result

See "Position Paper" attached.

Attachment

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.