

COOPOL and OPTICO Dissemination Event

12th September 2013, University of Hamburg
Technische und Makromolekulare Chemie
Bundesstraße 45
20146 Hamburg

Attendance by OPTICO and COOPOL consortium members only

Key outcome: knowledge transfer between
the OPTICO and COOPOL FP7 projects

Programme Booklet

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Agenda

09:00 – 9.15 Welcome and Introduction to the day

09:15 **Project Introductions**

9.15 – 9.30 OPTICO Project (*Prof. Costas Kiparissides, CERTH*)

9.30 – 9.45 COOPOL Project (*Prof. Alexei Lapkin, Cambridge*)

9.45 **Master Classes**

9.45 – 10.15 Emulsion Polymerisation
(*Klaus Dieter Hungenberg, BASF*)

10.15 – 10.45 The Current Status & Future Direction of Process Systems Engineering
– a Global Perspective
(*Prof. Stratos Pistikopoulos, ICL*)

10.45 – 11:00 Coffee Break

11:00 **Master Classes**

11.00 – 11.30 Advanced Modeling of Polymerization Processes
(*Prof. Costas Kiparissides, CERTH*)

11.30 – 12.00 On-line Sensors and Process Analytics Tools for Advanced Monitoring and
“Product Quality” Inference in Polymerization Processes
(*Dr. Suresh Thennadil, USTR*)

12.00 – 12.30 Nonlinear Model Predictive Control Technology for Improved Operation
of Industrial Scale Polymerization Reactors
(*Peter Singstad, Cybernetica*)

12.30 – 13.30 Lunch

13.30 **Poster session**

13.30 – 14.30 Poster display and Networking Session (with refreshments)

14:30 – 15.00 Poster Judging

15:00 – 15.15 Prize giving and Close

Master Class Summaries

Emulsion Polymerisation (*Klaus Dieter Hungenberg, BASF*)

COOPOL is about model-based intensification of polymerization processes – and emulsion polymerization is one of the most complex polymerization processes. So, successful intensification for this process should be easily transferable to other processes. After a general introduction to emulsion polymerization, the mechanism and the products from this process, the specific challenges for intensifying this process will be highlighted, and how the various contributions of the partners will solve these problems.

The Current Status & Future Direction of Process Systems Engineering – a Global Perspective (*Prof. Stratos Pistikopoulos, ICL*)

Process Systems Engineering focuses on the study and development of approaches, tools and techniques for modelling, analysis, design, optimization and control of complex process engineering systems. This presentation focuses on the current status of process systems engineering and highlights a number of future directions, both in terms of core competence areas and activities that constitute the ‘backbone’ of process systems engineering

Advanced Modelling of Polymerization Processes (*Prof. Costas Kiparissides, CERTH*)

Process modelling, optimization and control can have a significant impact on polymer plant operability and economics, however, it involves complex issues relating reaction mechanism, physical transport phenomena, mixing, reactor type and operating conditions to predict their affect on “polymer quality and properties”. To build robust modelling requires accurate data collection and interpretation from on-line monitoring instrumentation. The present paper deals with the advanced modeling optimization of particulate polymerization processes using a population balance approach.

On-line Sensors and Process Analytics Tools for Advanced Monitoring and “Product Quality” Inference in Polymerization Processes (*Dr. Suresh Thennadil, USTR*)

The extraction of information regarding particle size distribution and residual monomer concentration – two of the most important parameters in a suspension polymerization process using online spectroscopic measurements is considered. The methodology for using UV-VIS spectroscopy measurements to obtain particle size information under multiple scattering conditions through the use of the radiative transfer theory is described. Initial results from study of Raman measurements for extracting residual monomer concentrations are discussed.

Nonlinear Model Predictive Control Technology for Improved Operation of Industrial Scale Polymerization Reactors (*Peter Singstad, Cybernetica*)

Current applications for nonlinear model predictive control technology are fairly limited in number but typically yield increased profit margins through reduced product variability, reduced loss of production and better utilization of the production capacity. The presentation will review state-of-the art and present objectives for further developments in the COOPOL project including new methods and tools to demonstrate intensification of a semi-batch emulsion co-polymerization process. The activities include modelling for control, process identification, soft sensor development and robust strategies for dynamic real-time optimization.

Poster Titles

Process Modelling of Emulsion Copolymerization: Semi-batch & Smart-scale Reactor Simulation

Alexandr Zubov, Richard Pokorný, Fabian Lueth, Juraj Kosek

Dept. of Chemical Engineering, Institute of Chemical Technology Prague

Institute for Technical and Macromolecular Chemistry, University of Hamburg

Fouling of Emulsions: Modeling by Discrete Element Method

Martin Kroupa, Michal Vonka, Juraj Kosek

Dept. of Chemical Engineering, Institute of Chemical Technology Prague

Robust Model-based Control and Dynamic Real-time Optimization Methods

Jennifer Puschke, Adel Mhamdi, Alexander Mitsos, Wolfgang Marquardt

AVT - Process Systems Engineering, RWTH Aachen University

Soft Sensors for Semi-batch Emulsion Polymerization Process

Preet Joy, Adel Mhamdi, Alexander Mitsos, Wolfgang Marquardt

AVT - Process Systems Engineering, RWTH Aachen University

Online Monitoring of Emulsion Polymerisation

Claudia Houben, Gabit Nurumbetov, David M. Haddleton, Alexei A. Lapkin

Dept. of Chemical Engineering and Biotechnology, University of Cambridge and

Dept. of Chemistry, University of Warwick

Development of Advanced Reactor Systems for Emulsion Polymerisation

Gabit Nurumbetov, Claudia Houben, Alexei Lapkin, David Haddleton

Dept. of Chemistry, University of Warwick and

Dept. of Chemical Engineering and Biotechnology, University of Cambridge

Process Intensification of Continuous Emulsion Polymerization Reactions in Smart Scale PTFE Tubular Reactors

Fabian Lueth, W. Pauer, H.-U. Moritz

Institute for Technical and Macromolecular Chemistry, University of Hamburg

Multi functional Online Monitoring of fast Emulsion Polymerization with two different reactor concepts

Peter Bröge, Werner Pauer, Hans-Ulrich Moritz

Institute for Technical and Macromolecular Chemistry, University of Hamburg

Development of a Modelica Toolbox for Modeling of Emulsion Copolymerization Processes

Fredrik Gjertsen, Peter Singstad

Cybernetica Trondheim

On the Development of Advanced, Multi-Parametric Controllers for Nonlinear, Dynamic Processes

Maria Papathanasiou, Stratos Pistikopoulos, Sakis Mantalaris

Imperial College London

Suspension and Inverse-Suspension Polymerization Processes

Libor Šeda, Klaus-Dieter Hungenberg

BASF, Ludwigshafen

Estimation of monomer concentration in a suspension polymerization process using Raman spectroscopy

José García, Adel Mhamdi, Alexander Mitsos, and Wolfgang Marquardt
Process Systems Engineering, RWTH Aachen University

Estimation of particle size from spectroscopy measurements in EPS process

Maryam Ghadrhan, Adel Mhamdi, Wolfgang Marquardt, Alexander Mitsos
Process Systems Engineering, RWTH Aachen University

Process Intensification for the Purification of a monoclonal antibody

Fabian Steinebach, Marija Sarenac, Daniel Baur, Guido Ströhlein, Massimo Morbidelli
Institute for Chemical and Bioengineering, ETH Zürich and ChromaCon AG, Zürich

Compact Customisable Fibre-optic Multisensor System

Trevor Whittley, David Doig, Graeme Clifton Coles, Gary Colquhoun.
Fibre Photonics Ltd., Livingston

UFA oxidation with hydrogen peroxide

Markus Brandhorst, Jean-Luc Dubois
ARKEMA, Pierre-Bénite

On-line Sensors and Process Analytics Tools for Advanced Monitoring and “Product Quality” Inference in Polymerization Processes

Barry Robertson, Gillian Rundell, Yi-Chieh Chen, Suresh N. Thennadil, Alison Nordon, David Littlejohn
Dept. of Pure and Applied Chemistry and CPACT, Dept. of Chemical and Process Engineering, University of Strathclyde

Modeling of expandable polystyrene and polyacrylamide kinetics: Model accuracy and intrinsic kinetic parameters

Carolina Toloza Porras, William Scott Jr., Dagmar D’hooge, Marie-Françoise Reyniers, Guy Marin
Laboratory for Chemical Technology (LCT), Ghent University,

Modelling of the oxidation of Unsaturated fatty acids with hydrogen peroxide - A systematic approach

Marina Fedorova, Emmanouil Papadakis, Gürkan Sin, Rafiqul Gani
Computer Aided Process Engineering Center, Technical University of Denmark

Crystallization process for Pharmaceutical compounds

Fatemeh Anisi, Jeroen van Krochten, Stefan Goddrie, Richard Lakervard and Herman Kramer
Department of Process and Energy, Delft University of Technology

Experimental and Theoretical Kinetic Investigation of Particulated Polymerization Processes

Olympia Kotrotsiou, Chrysa Gkemetzoglou, Prokopis Pladis and Costas Kiparissides
Department of Chemical Engineering, Aristotle University of Thessaloniki and CERTH