Industrial Short Course: Robust Modeling in Process Optimization

August 4 - 5, 2015

OVERVIEW

Many industrial processes are based on chemical reactions in certain production environments including various species and particles from basic substances up to complex molecules like polymers, hydrocarbons or crystals. Detailed kinetic models are the most versatile way to describe the chemistry of these processes, which is necessary for the best possible understanding and an optimal chemical reactor design and control. Corresponding reaction networks easily contain hundreds of species and thousands of reactions, or even an a priori unknown number of species and reactions like in polymerization processes. Providing these networks with the required thermodynamic and kinetic data is one of the biggest challenges in chemical reaction engineering. Since experimental data are only available for a limited number of observables and their acquisition is still associated with significant cost and time, optimizing the kinetic models by fitting the model structure and model parameters to the available data is the key to reliable prediction of the process through simulations.

Moreover, complex models for polymers or related chain molecules consist of high-dimensional (population) balances and require particularly efficient and robust mathematical techniques. Even then, every individual simulation of a system already may produce considerable computational effort. Thus, advanced methods for parameter estimation in the context of model validation and improvement are essential for successful robust modelling in process optimization.

In order to address these issues with a focus on industrial applications, IPAM together with the German companies CiT (Computing in Technology), 8Berlin (www.8berlin.de), and the Research Campus MODAL offers a two-day short courseThe short course offers an introduction to the mathematical theory regarding uncertainty quantification, parameter estimation and model selection and validation. The resulting algorithms are discussed and applied to realistic examples from industrial research that include polymerization, degradation, aggregation and related processes in combination with associated reactor operation modes. This includes an introduction to the underlying model balances on day 1 and practical hands-on sessions using the advanced software package Predici on day 2.

SPEAKERS

Professor Dr. Christof Schütte: Christof Schütte is the vice president of the Zuse Institute Berlin (ZIB) and the Head of Biocomputing Group at the Freie Universität Berlin. His expertise includes mathematical modelling, simulation and optimization of complex systems in chemistry, biology and medicine. He has authored more than 150 cross-disciplinary scientific publications and has been an invited speaker at many international conferences, e.g., at ICIAM 2007 and ICM 2010.

Dr. Michael Wulkow: Michael Wulkow is involved in projects on the numerical treatment of processes in technical chemistry, biological chemistry and physics. He has given numerous international lectures at industrial companies, universities and workshops and has written publications in different fields. Michael Wulkow founded CiT in 1992, and currently serves as co-director of CiT. CiT's software packages (Predici Presto-Kinetics, Parsival) are used in most of the major chemical companies and in dozens of academic research institutes.

PARTICIPATION

The short course is for participants with scientific and technical background in the field of calibration or validation of mathematical models or model-driven data analysis in modelling, simulation and optimization of chemical processes. It is aimed at participants from the Chemical and Polymer Industry, Oil Industry, Pharma and Biotech Industry, Water Supply and Food Production. Topics will be adjusted depending on the exact interests of the participants.

The number of participants will be limited to 20. We will turn off registration when we reach capacity or by **June 4, 2015**, whichever comes first. Please register online at the link below and pay the $1000 registration fee early to ensure you have a seat. We encourage you to discuss your interest in the program with us before you register by sending us an email to isc2015@ipam.ucla.edu.

Location: Portola Plaza Building, UCLA

www.ipam.ucla.edu/isc2015