Modelling, Simulation and Parameter Estimation of Polymerization Processes

Berlin, 20th - 22nd November 2019

The **Research Campus MODAL** and **CiT GmbH** are glad to offer another workshop on **modelling**, **simulation** and **parameter estimation** of chemical reaction kinetics. The program combines lectures on **scientific topics** with introductory and advanced **tutorials** for CiT's program packages **Predici** 11.

Using mathematical models requires several tasks and a typical cycle should be undergone until a satisfying solution is found: choice and development of a **model** – realization in **software** – analysis of **simulation** results – identification of **parameters** - analysis of the quality of the fit – generation of more **data** or change of the model. Only then a robust **optimization** of the process can be done. None of these tasks is easy to perform. Models can be difficult to create, set up and maintain and hard to solve. Parameter estimation often adds a level of complexity that leads to challenging difficulties. Sometimes reasonable and unique parameters cannot even be found, sometimes it remains unclear, whether and why the whole model is or is not appropriate for the tasks under consideration.

The workshop describes the related techniques and addresses participants from industry and academia involved in the modelling and process optimization of chemical and polymerization kinetics. The workshop will present new and exemplary structures and will lead a way to further studies.

Venue: Zuse-Institute Berlin (**ZIB**), Takustraße 7, 14195 Berlin-Dahlem, Germany, www.zib.de

The language of the workshop will be **English**. Participants should bring their own **laptop** and will receive a time-limited, full working educational version of Predici for the exercises.

Fee: 850 € + VAT for industrial participants, 400 € + VAT for members of academic institutions.

Registration: The **registration** web site www.8berlin.de/KiMoPe2019Nov-Registration will be opened on Friday, October 18th. You may also directly contact Ms. Sandra Patzelt-Schütte, patzelt-schuette@zib.de or Michael Wulkow m.wulkow@cit-wulkow.de .

Lecturers:

Klaus-Dieter **Hungenberg** has been Vice President Polymer Reaction Engineering at BASF SE until his retirement in 2013. In 2012 he received an Honorary Professorship at the University of Paderborn. He is (co-)author of more than 100 scientific articles and patents.

Christof **Schütte** is the president of the Zuse Institute Berlin (ZIB) and professor for mathematics at the Free University Berlin. His research area is Scientific Computing with a strong focus on application problems from the life and material sciences.

Michael **Wulkow** founded the company Computing in Technology (CiT) in 1992 and since then has been involved in projects, research and numerous publications on the modelling and numerical treatment of processes in technical chemistry, biology, particle technology and pharmacokinetics.

Niklas **Wulkow** graduated in mathematics at the FU Berlin and is now PhD student in the field of applied Mathematics with emphasis on numerical analysis of stochastic memory exhibiting systems in the context of agent-based models.

Contents

Day 1: Wednesday, 20th **November**

9:15 am – 12:45 pm

- Basic kinetic modelling with Predici
- Reactor operation modes and recipes
- Basic concepts of user-defined scripts

1:30 am – 5:00 pm

- Overview on reaction mechanisms available in Predici
- Copolymerization and related topics
- Numerical background of Predici

Day 2: Thursday, 21st **November**

9 am – 12:30 pm

- Hybrid-Monte-Carlo simulations for polycondensation and radical copolymerization
- Parameter estimation – difficulties and challenges

1:15 pm – 5:00 pm

- Parameter estimation in Predici – exercises with Predici
- Parameter estimation – new approaches including the new Bayesian tool in Predici
- Modelling techniques and new features in Predici

Day 3: Friday, 22nd **November**

9 am – 12:30 pm

Open discussion, presentation of special models. Here we offer the opportunity to discuss advanced models and special user questions.

Of course, lunch and coffee breaks are included.

If there are any question regarding the contents, please contact:

Dr. Michael Wulkow, m.wulkow@cit-wulkow.de

K.-D. Hungenberg and M. Wulkow co-author the new book **Modeling and Simulation in Polymer Reaction Engineering** - A Modular Approach (ISBN: **978-3-527-33818-4**, Wiley-VCH, Weinheim)