



LEISTUNGSZENTRUM
SIMULATIONS- UND
SOFTWARE-BASIERTE
INNOVATION



INTERNATIONAL
PRESENCE WORKSHOP

**4TH MATHEMATICAL METHODS
IN PROCESS ENGINEERING –
MODELING, SIMULATION,
OPTIMIZATION**

October 5 – 6, 2023
Fraunhofer-Zentrum, Kaiserslautern

ENTRY FEES/REGISTRATION

– Entry fees

- Industry: 690 EUR*
(VAT is not charged according to § 4 No. 22a UStG)
Invoicing takes place after the event.
- Research staff: free of charge

*During the event, coffee, refreshments and lunch will be offered. Registered participants will receive workshop materials and can attend the networking dinner on October 5, 2023.

– Registration

Please register online by **September 22, 2023**:
<https://s.fhg.de/mmipe-2023>



GENERAL INFORMATION

– Contact with regard to scientific program

Prof. Dr. Michael Bortz
Department Optimization – Technical Processes
Fraunhofer Institute for Industrial Mathematics ITWM
Phone +49 631 31600-4532
michael.bortz@itwm.fraunhofer.de
www.itwm.fraunhofer.de

– Contact with regard to organization

Ilka Blauth
Phone +49 631 31600-4674
ilka.blauth@itwm.fraunhofer.de

– Conference venue

Fraunhofer Institute for Industrial Mathematics ITWM
Fraunhofer-Platz 1
67663 Kaiserslautern
www.itwm.fraunhofer.de

Directions: www.itwm.fraunhofer.de/contact

We acknowledge funding by Carl-Zeiss-Stiftung
and DFG/FOR 5359



PREFACE

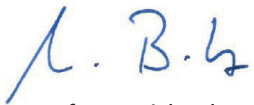
Model-based simulation and optimization is considered an essential ingredient for unveiling potential for increased energy and resource efficiency as well as for maintaining a high level of value creation.

Mathematical models, algorithms and data science are in the core of this development.

In fall 2023, October 5 – 6, the Fraunhofer High Performance Center Simulation and Softwarebased Innovation will organize the international workshop »Mathematical Methods in Process Engineering« with 6 internationally outstanding invited speakers and 12 short contributions from researchers of the center and industry.

All lectures are invited, and also attendance will require invitation.

The number of invited participants is limited to about 80, which will include selected partners from process industry as well. The workshop will provide a unique opportunity for scientific discussions and personal networking between scientists from academia and industrial practice to render and to shape the topics to come in future process engineering.



Prof. Dr. Michael Bortz
Fraunhofer ITWM



Prof. Dr. Hans Hasse
RPTU Kaiserslautern

PROGRAM – THURSDAY, OCTOBER 5, 2023

9:45	Registration open, welcome coffee
10:00	Opening Prof. Dr. Michael Bortz, Prof. Dr. Hans Hasse
10:15	Opening Keynote Dr. Alice Glättli, Senior Vice President, BASF SE
S1: MSO FOR DYNAMIC PROCESSES I Session Chair: Prof. Dr. Michael Bortz	
10:45	Some useful machine learning methods to support property prediction, molecule selection, and process design Prof. Dr. Kai Sundmacher, MPI for Dynamics of Complex Technical Systems
11:35	Expanding the solution space by ML-supported exploration of process simulation models Dr. Norbert Asprion, BASF SE
12:00	Solving robust optimization problems with a quadratic convergent adaptive discretization method: quADAPT Dr. Tobias Seidel, Fraunhofer ITWM
12:25	Lunch (foyer)
S2: PROCESS AND SHAPE OPTIMIZATION Session Chair: Dr. Dietmar Hietel	
13:30	Distillation: An old separation technique continues to innovate industries Prof. Dr. Thomas Grützner, Ulm University
14:20	Virtual Design of Catalyst Shapes and Fixed Beds Dr. Arne Hoffmann, BASF SE
14:45	Simulation-based Shape Design for Chemical Reactors Dr. Sebastian Blauth, Fraunhofer ITWM
15:10	Coffee break (foyer)
S3: PROCESS ENGINEERING Session Chair: Prof. Dr. Hans Hasse	
15:50	Optimization Modeling, Solution Strategies and Applications to Energy Processes Prof. Larry Biegler, PhD, Carnegie Mellon, Pittsburgh (USA)
16:40	The contribution of digital technologies to the energy transition from the perspective of Air Liquide Dr. Vanessa Gepert, AIR Liquide Forschung und Entwicklung GmbH
17:05	Modeling Unknown Mixtures Jun.-Prof. Dr. Fabian Jirasek, RPTU Kaiserslautern
17:45	Transfer via bus to our diner location For speakers and external industrial participants Round table discussions and networking dinner

PROGRAM – FRIDAY OKTOBER 6, 2023

8:30	Arrival of participants, welcome coffee
S4: SEPARATION AND PROCESS INTENSIFICATION Session Chair: Dr. Christian Leithäuser	
8:40	Multiphase flow in highly permeable media Prof. Michel Quintard, PhD, Toulouse INP (France)
9:30	Boundary conditions and tasks for modeling / simulation / optimization - an industrial perspective Dr. Thomas Runowski, Bayer AG
9:55	Modeling and simulation of transport processes in Ohmic reactors Dr. Sebastian Osterroth, Fraunhofer ITWM
10:20	Coffee break (foyer)
S5: MSO FOR DYNAMIC PROCESSES II Session Chair: Dr. Konrad Steiner	
10:50	Process synthesis and design of hybrid fluid separation processes Prof. Dr. Mirko Skiborowski, Hamburg University of Technology
11:40	Modeling, Simulation and Digital Transformation: How to manage Trust, Decision Making and Culture? Dr. Mattias Schmidt, Procter & Gamble Service GmbH
12:05	Multicriteria optimization opens up new perspectives on product portfolio design Dr. Helene Krieg, Fraunhofer ITWM
12:30	Lunch (foyer)
S6: SCHEDULING OF CONNECTED SYSTEMS Session chair: Prof. Dr. Karl-Heinz Küfer	
13:30	Digital Supply Chains: The Role of Advanced Optimization Techniques Prof. Ignacio Grossmann, PhD, Carnegie Mellon, Pittsburgh (USA)
14:20	The 20:80 approach: Using lean digital tools to enhance plant performance Dr. Daniel Staak, Arxada AG
14:45	Shape-constrained regression problems in engineering Dr. Jochen Schmid, Fraunhofer ITWM
15:10	Wrap up/closing
15:30	End of the workshop

Invited academic speakers

- Prof. Larry Biegler, PhD, Carnegie Mellon, Pittsburgh (USA)
- Prof. Ignacio Grossmann, PhD, Carnegie Mellon, Pittsburgh (USA)
- Prof. Dr. Thomas Grützner, Ulm University
- Prof. Michel Quintard, PhD, Toulouse INP (France)
- Prof. Dr. Mirko Skiborowski, Hamburg University of Technology
- Prof. Dr. Kai Sundmacher, MPI Magdeburg